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A CRITICAL REVIEW OF THE NUMERICAL SOLUTION OF NAVIER-STOKES EQUATIONS

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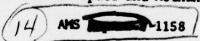
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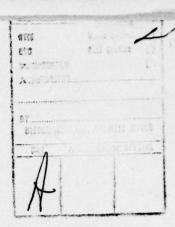


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A CRITICAL REVIEW OF THE NUMERICAL SOLUTION OF NAVIER-STOKES EQUATIONS

by

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I. INTRODUCTION

This article concerns the various practical problems of using high speed electronic computers to obtain approximate solutions of various fluid flow problems, not with the mathematical techniques of solving the Navier-Stokes equations through difference approximations in generality. The boundary conditions are as important as the partial differential equations in the mathematical formulation defining a given physical problem. There are complicated practical problems of discretizing the differential formulation (of both the differential equations and the boundary conditions) into appropriate difference formulation for its numerical solution. There are quite a few unusual aspects in such attempts.

Fluid dynamicists usually ignore the question of convergence in the asymptotic differential approximations through perturbation arguments.

They often consider the computational solution of the resulting system of ordinary differential equations, as routine, even though it may be

very tedious, and often iil posed especially for the multi-eigen-value problems. Under difficult circumstances, heurisite local treatments are often introduced to remedy the situation, or a slightly different original approach will be employed. Such a hit and miss approach has been carried over to the direct computational solution of the partial differential equations system of fluid dynamics. They lead to much more disappointment and often times with more serious consequences. While it may not be crucial to approciate the mathematical details, it is important to be aware of the implications of some fundamental mathematical results concerning the difference approximations of a partial differential equation. Accordingly, a brief review of these mathematical aspects will be outlined prior to the discussion of the practical art of numerically integrating the partial differential equations system of fluid dynamics.

Within the continuum description, the fluid will be considered to be homogeneous and to possess two independent thermodynamic, or state variables, i.e., the density ρ and the internal energy e per unit mass. There is an algebraic equation of state, relating the thermodynamic pressure p to its density ρ and internal energy e as $p = p(\rho,e)$. Let u_i be the velocity vector of a fluid element with i = 1,2 and 3 in a three-dimensional space x_i . u_i , ρ , and e are the five dependent variables and will be considered as functions of x_i and t. The Eulerian description of the change of these dependent variables, is the set of five partial differential equations, expressing the conservation of mass momentum and energy written here in divergence form as:

$$\frac{\partial \rho}{\partial t} + \frac{\partial}{\partial x_j} \left[\rho u_j \right] = 0 \tag{1.1}$$

$$\frac{\partial(\rho u_i)}{\partial t} + \frac{\partial}{\partial x_j} \left[\rho v_i u_j + p \delta_{ij} - \tau_{ij} \right] = 0$$
 (1.2)

$$\frac{\partial(\rho e)}{\partial t} + \frac{\partial}{\partial x_i} \left[\rho u_j \left(e + u_i u_i / 2 \right) + \rho u_j - q_j - u_i \tau_{ij} \right] = 0$$
 (1.3)

When the surface stress τ_{ij} is related linearly to the strain rate as

$$\tau_{ij} = \mu(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}) + (\kappa - \frac{3}{2}\mu) \frac{\partial u_j}{\partial x_j}$$
 (1.4)

and when the heat transfer vector q, is linearly related to the temperature gradient as

$$q_{j} = -k \frac{\partial e}{\partial x_{j}} = -\frac{\gamma}{Pr} \mu \frac{\partial e}{\partial x_{j}}$$
 (1.5)

the system of equations (1.1-1.3) will be referred to as the Navier-Stokes equations for a compressible fluid. The Prandtl number Pr and the specific heat ratio γ are properties of the fluid and are both of O(1). The shear viscosity coefficient μ is assumed to be a known algebraic function of temperature (or internal energy). The bulk viscosity coefficient is

often taken as zero or otherwise absorbed in μ . In dimensionless form a Reynolds number may be defined in terms of some characteristic length L_0 and velocity U_0 as $Re_0 = \rho_0 U_0 L_0/\mu_0$ where subscript o indicates that the quantity is to be evaluated at some reference state. For most fluid dynamics applications, the Reynolds number is very large.

The divergence form of the Navier-Stokes equations (1.1)-(1.3) may be written as

$$\frac{\partial v}{\partial t} + \frac{\partial}{\partial x_i} F(v, \frac{1}{Re} \frac{\partial v}{\partial x_k}) = 0$$
 (1.6)

posed as an initial value problem for the vector unknown v, having the five scalar components ρ , ρu_i , and e. F is the flux of v, given by the nonlinear quantities in the square brackets of Equations (1.1)-(1.3). When physically meaningful, initial and boundary data are prescribed, Equation (1.6) is expected to give a satisfactory description of the temporal development of the flow field at later times. This expectation is mathematically justifiable. The integration of this equation's system is needed, for example, in weather forecasting and in the determination of the temporal development of blast waves, hurricanes, or turbulent fluctuations, etc. (where the gravitational field and the coriolis forces are included where necessary). In most aeronautical applications, the steady state (or the quasi-steady state) problems are more often of primary interest where the temporal dependence is neglected. Thus Equation (1.6) becomes

$$\frac{\partial}{\partial x_j} F(v, \frac{1}{Re} \frac{\partial v}{\partial x_k}) = 0$$
 (1.7)

which is to be solved as a boundary value problem. The boundary conditions must, of course, be independent of time. But it is not clear how such boundary conditions should be specified to provide the required steady state solution or, indeed, any solution at all. Physical intuition often provides meaningful guidance but not all what is needed.

The stress and the heat conduction terms give rise to the second and the highest order partial derivatives with coefficients proportional to Re⁻¹. This steady state Navier-Stokes Equation (1.7) generally assumes an elliptical behavior. When Re becomes large, the flow field may be divided into sub-regions. In the region sufficiently far away from any solid boundary, the inviscid approximation, obtained by dropping terms in (1.6) or (1.7) containing Re⁻¹, is a valid approximation, known as the Euler's Equation

$$\frac{\partial \mathbf{v}}{\partial t} + \frac{\partial}{\partial \mathbf{x}_j} \mathbf{F}(\mathbf{v}) = 0 \tag{1.8a}$$

$$\frac{\partial}{\partial x_j} F(v) = 0 \tag{1.8b}$$

The time dependent inviscid Equation (1.8a) remains hyperbolic and is posed as an initial value problem as is Equation (1.6). The steady state Equation (1.8b), however, can be purely elliptic (subsonic) or purely hyperbolic (supersonic) or mixed, (i.e., with both elliptic and hyperbolic regions, the boundary of which will depend on the solution and are not known before hand such as in the supercritical transonic inviscid flow problem).

In the regions near the solid boundary, or near where there is a large shear stress or heat conduction, some or all of the stress terms contained in $F(v, \frac{1}{Re} \frac{\partial v}{\partial x_k})$ have to be kept with the other terms despite the large Re. If this viscous region should extend along a coordinate surface (x_1, x_2) such that the lateral extent (along x_3) of this viscous layer is small compared with its physical extent along the (x_1, x_2) surface, then Prandtl's boundary layer theory applies. Only the highest

order partial derivative in this lateral direction $(\partial^2/\partial x_3^2)$ will survive the limit of very large Re. This asymptotic limit at large Re gives the boundary layer equations which are parabolic. However, not all viscous layers are sheet like and can be treated by Prandtl's boundary layer approximation. For such viscous layers like the near wake and the interaction region between a shock wave incident on a boundary layer, the full Navier Stokes Equation (17) will have to be used and the problem becomes elliptic at least in a significant portion of the flow field of interest.

The change of the mathematical character of the flow field in different regions when the Reynolds number is large is both a blessing and a cause of concern. It is a blessing that enabled the development of fluid dynamics, historically, in the form of the inviscid or perfect fluid theory and of the boundary layer theory. But it is also the fundamental difficulty in the analysis of the mixed flow regions, characteristic of most of interaction flow problems. Now there are significant differences in the numerical integration of the three types of partial differential equations. The mathod that has been proved to be successful for one type need not be so for the other. It is therefore important to recognize the type of the partial differential equation before formulating a difference approximation for its numerical integration. Clearly then there are difficulties in the numerical integration of mixed problems. Such difficulties are quite different from those encountered in the asymptotic analysis of mixed flow problems. In a few examples, they have been successfully resolved with appropriate cautionary measures. But there is no theorem to guarantee its success in other problems.

It might be asked that if the elliptic steady state Navier-Stokes Equations (1.7) could be integrated for a given finite but large Re, why should the difficulties arising from the asymptotic limit of Re + \infty concern us. An obvious answer may be that the asymptotic form of the partial differential equations system is much simpler. A more fundamental reason is that, at finite but large Reynolds numbers, the asymptotic behaviors of the flow in different regions bear strongly on the appropriateness of the difference formulation and the numerical integration of the Navier-Stokes equations when the resolution (or the number of meshes per linear dimension of the field of computation) is severely limited.

For a flow problem in three space dimensions, an average of 30 meshes per linear dimension will give rise to 3 x 104 nodel points; and will need 1.5 x 105 words of storage spaces for the 5 unknowns at each point. Such storage spaces should preferably be provided in the core of the computer unit for ready access. Such a requirement will stretch the core memory capacity of most of the currently available large computers such as CDC 6600 or IEM 360-91. The solution of the full Navier Stokes Equation (2.7) for a well-posed boundary value problem will need hours of computation in such machines. The parallel computers in the stage of advanced development like ILLIAC IV and the STAR, can neither promise much improvement in this regard. To extend the core memory capacity, a hierarchy of external storages will be provided. Frequent reference to such external storages, however, will greatly increase the time required for data management because of the slow input-output devices connected to the central processing unit. This problem is particularly aggravated in the aforementioned parallel computers where the promised large gain in arithematic speed can be obtained only for specific modes

of "parallel" or "vector" computations in which a huge amount of data must be properly processed and continuously fed into the arithmatic unit(s).

The concept of parallel use of an array of mini-computers might appear to relieve such a difficulty associated with the specific mode of high speed arithematic operations. The benefit is likely to be illusory, however, at least for the present applications. It simply transfers onto the users the tremendous problem of optimal coordination of the operations of the array of mini-computers and the problem of data management among the diversed "internal" and "external" storage facilities. The users are ill-equipped with the expertise of the computer scientists who designed the softwares managing the businesses of the central procassing unit of the large computers. The users will be left to derive whatover speed advantage each individual program may provide. It should be remembered that without the order(s) of magnitude increase of the "overall processing speed" of the computer(s), the increase in the number of mesh points in a linear dimension for the integration of a problea can easily escalate the computer processing time from hours to days and months. It appears, even projected slightly into the future, that no more than a couple of hundred mesh points per linear dimension can possibly be considered in the integration of the system of equations of fluid dynamics. With such a limitation on the resolution of computational solutions, the integration of the full Navier-Stokes equation for the flow field over a vehicle, for example, (the external flow problem) seems futile. The field of computation is much like the test section of a windtunnel. Without the "full scale" facility, computers, like windtunnels, should be used at present to study only the components or the

local flow fields. For such purposes, various asymptotic forms of the Navier Stokes equation's system should be used for different parts of the flow field. The full Navier-Stokes equation's system will be called upon only for the study of those flow problems that cannot be consistently treated with the simplified flow equations, including notably those mixed interaction flow problems. Under the practical limitations of resolution and of computer time, it is particularly important to delineate the varying nature of the flow regimes in the different treatments of the Navier-Stokes equations and to consider the various possibilities of how the boundary conditions may be implemented. To quote the 1960 statement of Forsythe and Wasow: "The numerical solution of partial differential equations is no easy matter. Almost every problem arising out of the physical sciences requires original thought and modifications of existing methods". This statement is equally true today, and particularly so for the type of flow problems under consideration here.

II. FUNDAMENTAL CONCEPTS

Consider now the problem of solving a partial differential equation subject to a set of initial and boundary data through numerical integration. A difference formulation is obtained by replacing the differential coefficients by appropriate difference quotients as an approximation to the differential problem. There will be some "errors" in the approximate formulation both in the equation and in the initial and boundary data. When these "errors" vanish as the mesh sizes $\Delta t \rightarrow 0$ & $\Delta x \rightarrow 0$ in some manner, the difference approximation is said to be "consistent" with the differential problem. The solutions of this difference formulation provide a sequence of approximate solutions, which, in the limit of Δt , $\Delta x \rightarrow 0$, is supposed to "converge" to the solution of the differential problem in some sense; i.e., the "error" of the solution, as a measure of the departure of each member of the sequence of approximate solutions from the solution of the differential problem, tends to "zero". This convergence is, however, not guaranteed for a consistent approximate difference formulation. Various aspects will be considered in the following sections.

2.1 Well-Posed Differential Problem

The differential problem should not only possess a unique solution, but also possess "neighboring solutions", whether the problem is to be integrated analytically or numerically. This means that when the initial-boundary data is slightly perturbed, the differential problem should still provide a solution, which hopefully, departs from the unperturbed solution of the problem only slightly. This is primarily a physical requirement

expounded by Hadamard if a mathematical problem is to describe a physical situation appropriately. Mathematically speaking the solution of the differential problem is said to vary continuously with the data; and the differential problem is said to be "well posed". Among other things, a given partial differential equation is well posed only when the boundary conditions are properly specified. For example, the Laplace equation, in two variables x and y,

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0 \tag{2.1}$$

is well posed when the values of the function u(x,y) is specified on a closed boundary enclosing the domain of x,y of interest, (Dirichlet Problem). Now the function

$$u(x,y) = n^{-\alpha} \sin nx \cosh ny \qquad (2.2)$$

is an exact solution of the Laplace equation with the initial data

$$u(x,0) = n^{-\alpha} \sin nx$$

$$\frac{\partial u}{\partial y}(x,0) = 0$$

This set of initial data is small everywhere on x with $\alpha > 0$ and n sufficiently large. Now if the Laplace equation is to be solved when u(x,0) and $\frac{\partial u}{\partial y}(x,0)$ are specified, then a small perturbation of the initial data can introduce the perturbations of the type (2.2) onto the solution of the problem. This perturbation (2.2) is not small in the immediate neighborhood of y = 0 despite the small error of the initial data when n is large and α is positive. While the perturbation (2.2) does vanish at y = 0 for any

value of n including $n + \infty$, the value of u(x,y) given by (2.2) at some small but finite value of y, becomes infinitely large as $n + \infty$. Thus the Laplace equation is not "well posed" or "ill-posed" when u(x,0) and $\frac{\partial u}{\partial y}(x,0)$ are specified, (Cauchy Problem). If we should proceed to integrate this "ill-posed" problem, the perturbed initial data is expected to contain components like $Q \cdot Q$, and the numerical solution will not converge to the desired solution even if $\Delta x + 0$ (i.e., $n + \infty$).

If the gradient of u(x,y) is specified over a closed boundary (Neumann **Problem**) or if either the gradient or the value of u(x,y) is specified over a closed boundary, the problem of solving the Laplace equation is well posed if some integral conditions are met. Ill-posed problems will result otherwise, i.e., either when the Dirichlet or Neuman conditions are specified only on an open boundary, or when the Cauchy condition is used anywhere. This statement is applicable to elliptical partial differential equations in general. The parabolic equations are well posed under similar conditions but only on an "open" boundary and when integrated in the "positive" direction. The hyperbolic problems are well posed only when the Cauchy conditions are specified on appropriate "open" portion of the boundary. It becomes then difficult to specify the boundary conditions that will render a mixed differential problem well posed before attempting to formulate a difference approximation of the problem for numerical integration. From this point of view, the algebraic complexities of the full Navier-Stokes equations system, either for the time dependent hyperbolic problem (1.6) or for the steady state elliptical problem (1.7), may well be tolerated to facilitate the formulation of a well-posed problem.

2.2 Well-Posed Difference Problem

It is not only that the differential problem should be well posed for a specific or a selected class of initial data, but also that the difference problem should be well posed and, for a more general class of initial data, to provide a convergent numerical solution. This is because the perturbations implicit in the numerical solution of the approximate difference formulation need not fall within the class of the initial data for which the differential problem is well posed. The function

$$u(x,t) = \exp [i\alpha(x+t)]$$
 (2.3)

satisfies the first order hyperbolic equation

$$\frac{\partial}{\partial t} u - \frac{\partial}{\partial x} u = 0 \tag{2.4}$$

with the initial value

$$u(x,0) = \exp(i\alpha x)$$
.

The complex notation with $i = \sqrt{-1}$ is used here for simplicity, to mean that both the real and the imaginary parts of the expressions should be valid simultaneously. A wide class of function u(x,0) can be formed by superposing various trigonometric initial data corresponding to various choices of the values of the constant α . Each component can possess an arbitrarily assigned amplitude. By summing up the component solutions of different α 's, the solution of the problem with the generalized initial data is obtained. Any numbers of the component solutions can be perturbed with a correspondingly small perturbation on the solution. The differential problem is thus well posed.

Suppose now the forward time centered space difference algorithm is used to provide a difference approximation to (2.4) as:

$$\frac{U_j^{n+1} - U_j^n}{\Delta t} = \frac{U_{j+1}^n - U_{j-1}^n}{2\Delta x}$$

$$U_j^o = \exp(i\alpha x)$$
(2.5)

where $U_{\mathbf{i}}^{\mathbf{n}} = U(\mathbf{j}\Delta \mathbf{x}, \mathbf{n}\Delta \mathbf{t})$.

An exact solution of the difference problem (2.5) is

$$U_j^n = U(j\Delta x, n\Delta t) = (1 + i \frac{\Delta t}{\Delta x} \sin \alpha \Delta x)^n \exp(i\alpha x)$$
 (2.6)

where $n = t/\Delta t$. In the limit of $\Delta t \to 0$ & $\Delta x \to 0$, the difference solution U_j^n , given as (2.6), converges uniformly to the solution u(x,t), given as (2.3), for the differential problem (2.4). The same holds true for all the components and for their sum with a generalized initial data. Now when the difference problem (2.6) is computed for any small Δt and Δx , the computation is always unstable (as is well known). It is apparent that some components of the perturbations introduced by the computation of the difference form (2.5) cannot be represented by the trigonometric data and grow out of bounds.

The Euler's equation (1.8a) for inviscid gas dynamics is easily cast into Cauchy-Kowaleski type quasi-linear hyperbolic equations system

$$\frac{\partial u}{\partial t} + A(u) \frac{\partial u}{\partial x_j} = 0, \qquad (2.7)$$

where $A(u) = \frac{\partial F}{\partial u}$. If the initial data of u(x,t=0) = f(x) and A(u) are analytic, then the solution u(x,t) for all x and t is analytic. The requirement of the analyticity of the initial data might not appear to

True that any continuous function within a closed interval can be approximated arbitrarily closely by analytic functions, including polynomials and sinusoidal functions. But arbitrarily close approximation of the initial data does not promise the arbitrarily close approximation of the solution. The two examples (2.1) and (2.5) given above illustrate this point both for the differential and the difference equations.

Equation (1.8a) or (2.7) for inviscid gas dynamics is a well-posed problem for a fairly broad class of initial data. Even if it is presumed that a consistent difference approximation possesses a solution that converges uniformly to the solutions of the differential problem, stable computation is not guaranteed. The instability of the computation is attributed to the fact that the perturbations on the initial data introduced by the computational procedure is beyond the class of perturbations expressible in terms of the piecewise analytic data. For a difference problem to be well posed, its solution must be continuous with a much wider class of perturbations on the initial data. This is the crux of the concept of computational stability.

Computational stability in general calls for the boundedness of all the perturbations in the computed solution. Then when the magnitudes of the perturbations in the initial data are made arbitrarily small in the limit of vanishingly small mesh sizes, the resulting perturbations in the computed solution will likewise vanish. The computed neighboring solutions based on a consistent difference formulation will then converge to the solution of the differential problem; i.e., stability and consistency

means convergence. This is the essence of the equivalence theorem of

Lax. The success in obtaining a convergent approximate solution through

the computation based on a given difference formulation therefore lies in:

- (i) the consistency of the difference formulation with the well-posed differential problem,
 - (ii) the stability of the difference formulation.

Here, the difference formulation means collectively all the difference relations connecting the values of functions at different time levels and at all the mesh points in the interior of and on the boundary of the field of computation.

2.3 Computational Stability

Computational stability is a characteristic of a set of difference equations, not of a difference algorithm how a differential coefficient in the differential equation is to be replaced by a difference quotient. It is incorrect to refer to an algorithm as stable or unstable. The same algorithm when applied to different differential equations can lead to different difference equations with entirely different stability characteristics. Thus, the forward time and centered space difference algorithm when applied to the simple wave equation (2.4) leads to an always unstable difference equation (2.5). When the same algorithm is applied to the heat diffusion equation, the resulting difference equation is stable if $s = \frac{\Delta t}{\Delta x^2} < \frac{1}{2}$. Some simple examples are given in Tables I and II.

Slightly different algorithms, applied to the same differential equation may yield difference equations with quite different stability behavior. For the simple wave equation (2.4), the forward time and the backward space difference algorithm will yield an always unstable difference

$$L(u) = (\frac{\partial}{\partial t} + c \frac{\partial}{\partial x}) u = 0$$

	$L_{\Delta}(u)$ WITH $r = c \frac{\Delta t}{\Delta x} > 0$	e₁ = L∆(u)-L(u)	STABLE
=	(uj+'-uj)+ r (uj+r-uj)	O(∆t, ∆x)	UNSTABLE
2)	(uj+1-uj) +r (uj-uj-1)	O(\Dt, \Dx)	IF r ≤ 1
3	$(n_{j+1}^{n-1}-n_{j}^{n})+\frac{\Gamma}{2}(n_{j+1}^{n}-n_{j-1}^{n})$	O(\Dt, \Dx^2)	UNSTABLE
4	4)	0(∆t, ∆x²)	F r A
2)	un-1-0,-1 + r (un-1-1,-1)	0(\D12,\Dx^2)	ALL, r
	MOST IMPLICIT SCHEMES		ALL r

TABLE I

	$L(u) = (\frac{\partial}{\partial t} - \nu \frac{\partial^2}{\partial x^2}) u = 0$	$v\frac{\partial^2}{\partial x^2} \mid u = 0$	
	L∆(u) WITH S=V ^{∆†} /∆x²	(n)-۲(n) [∇] 7 = +0	STABLE
=	(1-ln+l-nl) - 2(nl+1-2nl+nl-1)	(∆†,∆ײ)	F s ≤ ½
2	2) $(u_j^{n+1} - \frac{u_{j+1}^n + u_{j-1}^n}{2}) - s(u_{j+1}^n - 2u_j^n + u_{j-1}^n)$	0(Δt, Δx²)	UNSTABLE
33	3) (uj+'-uj-')-2s(uj+r2uj+uj-1)	$O(\Delta t^2, \Delta x^2)$	UNSTABLE
4	4) (uj -uj -2s(uj -uj -uj -uj +uj-1)	0(\Dis , \Du \cdot 2)	ALL S
•	MOST IMPLICIT SCHEMES		ALL S

TABLE II

equations

$$\frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} - C \frac{U_{j}^{n} - U_{j-1}^{n}}{\Delta x} = 0$$
 (2.8)

The forward time and the forward spatial difference algorithm will provide the difference equation

$$\frac{v_{j}^{n+1} - v_{j}^{n} - v_{j+1}^{n} - v_{j}^{n}}{\Delta x} = 0$$
 (2.9)

that will be stable if $C \Delta t/\Delta x \le 1$. And, as mentioned previously, the forward time and centered space difference algorithm, Equation (2.5), is always unstable. The choice of difference algorithm for discretization to obtain a stable difference equation is not trivial.

For a slightly more complicated equation, the situation is considerably more complex. A partial differential equation of higher order may be written as an equivalent system of lower order partial differential equations. (Contrary to the situation of higher order ordinary differential equations, this is not generally true for partial differential equations). A partial differential equation representing a physical principle may be written in different but equivalent forms in terms of different subsidiary variables. When the same difference algorithm is applied to discretize these equivalent differential forms, the resulting difference equations are not equivalent and may possess widely different stability behavior in computation. Consider the simplest case of the second order wave equation

$$\frac{\partial^2 \phi}{\partial t^2} = C^2 \frac{\partial^2 \phi}{\partial x^2} \tag{2.10}$$

which is equivalent differentially to a system of two first order wave equations. We may write the system in terms of different variables as:

$$\begin{cases} \frac{\partial \phi}{\partial t} = v \\ \frac{\partial v}{\partial t} = C^2 \frac{\partial^2 \phi}{\partial x^2} \end{cases}$$
 (2.11a)

and

$$\begin{cases} \frac{\partial \mathbf{v}}{\partial t} = \mathbf{c} \frac{\partial \mathbf{u}}{\partial \mathbf{x}} \\ \frac{\partial \mathbf{u}}{\partial t} = \mathbf{c} \frac{\partial \mathbf{v}}{\partial \mathbf{x}} \end{cases}$$
 (2.11b)

When forward time and centered space difference algorithm is used, the following difference equations system results

$$\begin{cases} \frac{\phi_{j}^{n+1} - \phi_{j}^{n}}{\Delta t} = V_{j}^{n} \\ \frac{V_{j}^{n+1} - V_{j}^{n}}{\Delta t} = C^{2} \frac{\phi_{j+1}^{n} - 2\phi_{j}^{n} + \phi_{j}^{n} - 1}{\Delta x^{2}} \end{cases}$$
(2.12)

and

$$\begin{cases} \frac{V_{j}^{n+1} - V_{j}^{n}}{\Delta t} = C \frac{U_{j+1}^{n} - U_{j-1}^{n}}{2\Delta x} \\ \frac{U_{j}^{n+1} - U_{j}^{n}}{\Delta t} = C \frac{V_{j+1}^{n} - V_{j-1}^{n}}{2\Delta x} \end{cases}$$
(2.13)

The system (2.12) is always unstable for any choices of Δt and Δx (easily verified by v. Neumann Analysis) while the system (2.13) is stable if $C \Delta t/\Delta x \leq 1$. Note also that the similar difference equation (2.5) for the first order wave equation (2.4) is always unstable. Thus, it is not a matter of trivial consequence to rewrite a partial differential equation into equivalent but different forms before discretization with the same difference algorithm.

The equations of fluid dynamics represent the three conservation laws of mass, momentum and energy. They can be expressed in terms of

a great number of dependent and independent variables or in terms of particular combinations of such variables and in different coordinate systems. The second order equations may be split into first order systems. (For the moment, the question of nonlinearity is put aside.) For all these varied forms of equivalent systems of partial differential equations (equivalent in the sense of physics and mathematics) a given difference algorithm will give correspondingly varied difference forms with quite different stability and other computational behaviors.

The complete difference formulation of a fluid dynamics problem will call for the discretization of the boundary condition in addition to the set of differential equations. The set of difference relations connecting the values of various functions at mesh points neighboring the boundary is generally different from the set of recursive relations for the interior points derived from the differential equations. This boundary set of difference relations may be unstable while the recursive difference relations for the interior points are stable. Apparently trivial modifications of the difference formulation in the boundary conditions thus often lead to substantial changes in the stability behavior.

In view of such a complicated situation and of the frequent experience of severe computational instability, it it highly desirable to be able to analyze the stability behavior of a given difference formulation; but there is no simple means available except the so-called "energy analysis". The "energy analysis" attempts to establish a finite bound of the solution (over the entire net or mesh space) in some suitably-chosen norm, and the formulation is by definition stable. When such a bound is established, the proof of convergence, existence, and uniqueness follows trivially. For a nontrivial boundary value problem, such a proof is very

difficult and very tedious even for a simple equation. Such proofs are available for the Navier-Stokes equations for an incompressible fluid, but only for the periodic boundary conditions, a case which is really not that much different from a pure initial value problem. With rather complicated boundary conditions, it is not practical if not impossible, to ascertain the stability property of a difference formulation of a fluid dynamics problem via such an approach. At present, it is a practical art to draw from experiences with similar problems and inferences of model analysis in formulating the recursive difference relations for the interior points. The formulation of the boundary conditions is approached on an individual basis and modified where necessary. The entire program is then tested in actual computer computation for its stability. Considerable work will be involved before stable computation is achieved. By then quite a few modifications may have been introduced. It is opportune to check if the final difference formulation is consistent with the differential problem to be solved both as to the differential equations and the boundary conditions.

It may well be that the physical boundary conditions that should be applied are quite different from those consistent with the difference formulation or that some spurious terms might have been introduced into the differential equations that fail to vanish in the limit of Δt , $\Delta x \to 0$. The v. Neuron stability analysis for the local linearized model will most likely impose some restrictions on Δt and Δx for the computation to remain stable. This restriction should be observed by all the approximate solutions, as successive members in the Cauchy sequence, converging toward the solution of the differential problem. The limit process in the t-x space is not to be taken in any arbitrary manner. This restriction should be considered while investigating the consistency of the difference formulation.

Certain difference algorithms are often referred to as "unconditionally stable". What it means is that when such an algorithm is used to discretize a certain type of differential equation for the solution of pure initial value problems or of periodic boundary value problems, there will not be restrictive conditions on the choice of Δt (or of the iterative steps in the solution of pure boundary value problems) for a given set of Ax, according to the v. Newman stability analysis of the linear equations. When such an algorithm is used in the numerical solution of non-periodic boundary value problems, even for that particular type of equations, computational instability will often result especially for complicated boundary conditions and for non-linear equations. Even if no question of stability arise, the apparent advantage of permitting the use of too large time steps At need not lessen the computing time while inevitably decreases the accuracy of the computed solution. Indeed it is advisable under the circumstances to verify the consistency conditions for both the equation and the boundary condition.

A case to illustrate the point is the following. The integration of the simple heat diffusion equation

$$\frac{\partial \mathbf{u}}{\partial \mathbf{t}} = \frac{\partial^2 \mathbf{u}}{\partial \mathbf{x}^2} \tag{2.14}$$

with the formally second order accurate, centered time, centered space algorithm of DuFort-Frankel:

$$\frac{U_{j}^{n+1} - U_{j}^{n-1}}{2\Delta t} = \frac{U_{j+1}^{n} - 2U_{j}^{n} + U_{j-1}^{n}}{\Delta x^{2}} + \frac{U_{j}^{n+1} - 2U_{j}^{n} + U_{j}^{n-1}}{\Delta t^{2}} \left(\frac{\Delta t}{\Delta x}\right)^{2}$$
(2.15)

is "unconditionally stable" for any positive values of $s = \frac{\Delta t}{\Delta x^2}$ so that Δt can be made as large as Δx or larger without leading to computational

instability. Most other explicit difference algorithms when applied to the heat diffusion equation will impose a stability limit like $s \le \frac{1}{2}$. The restriction on Δt is particularly severe at small Δx . Now, in integrating Equation (2.15), it is tempting to use as large a Δt as is practical, usually comparable to Δx , to save computing time. Indeed, this is often credited as the "merit" of the Dufort-Frankel scheme. Equation (2.15) is, however, consistent with the heat diffusion equation only when $\frac{\Delta t}{\Delta x} + 0$ as $\Delta x + 0$. Otherwise, it is consistent with the wave equation, having the wave speed $\frac{\Delta x}{\Delta t}$.

$$\left(\frac{\Delta t}{\Delta x}\right)^2 \frac{\partial^2 u}{\partial t^2} + \frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}$$
 (2.15a)

With $\frac{\Delta t}{\Delta x}$ = O(1), the computed solution is expected to display waves comparable to the temporal and the spatial variations of the solution, and therefore loses much of its value as an approximation to the solution of the diffusion problem (2.14). Even with $\Delta t/\Delta x^2$ = s \leq 1/2 for example, the computed solutions will still display oscillations, albeit at smaller amplitudes. The mean solution (taken over the waves) is neither a meaningful approximation of the solution to the diffusion problem with Dirichlet boundary conditions. If a Neuman boundary condition should be imposed, instability will result. The qualitative statements mentioned here should not be generalized. The simple example is given above only to bring home the point that every individual problem should be carefully examined according to the fundamental principle. Our current understanding of the numerical integration of the partial differential equations does not warrant any simple generalization to be applied to the complicated situations of fluid dynamics.

III. STABILITY ANALYSIS

The numerical integration of the Navier-Stokes Equations, as an outstanding example of complicated partial differential equations system is expected to encounter quite serious practical difficulties. Such difficulties fall into three basic categories which may not be all independent:

- (i) Computational Stability All disturbances will remain bounded in the computation. Otherwise, the value of some quantity will eventually become so large as to be beyond the capability of any computer and no results would be obtained. Hence, this is often referred to as computability.
- (ii) Convergence Rate The solution at some later time T or at the asymptotic steady state should be obtained with a reasonable amount of computational work, i.e., the number of time or iterative steps in the solution must not be too large and the computational work for each step not excessive so that results can be obtained within a reasonable amount of time (and hence cost).
- (iii) Accuracy The solution eventually obtained must in some sense approximate the physical results in question for it to be useful. The criterion for its being an adequate approximation is, however, subject to judgement. The accuracy criterion imposes limitations on the fineness of the resolution, both temporally and spatially, which in turn sets the requirement on the convergence rate.

Computational stability is clearly the most pressing problem, since it is the first one to be encountered in an attempt to get any solution. Much work has been devoted to this question. As is explained in the previous chapter, its fundamental nature is essentially understood but there are quite a few subtle aspects in its implementation even for the simple

examples. The practical question of achieving a stable computation for the complicated system of Navier-Stokes Equations is expected to be formidable. The various heuristic approaches that promise to guide the formulation of a stable difference problem will be reviewed in the following chapter. Generally speaking, with some hard work, stable computation can usually be achieved as may be verified in actual computation. It is important, however, at this juncture to bear in mind that the convergence rate and the accuracy of the formulation should not be seriously compromised in an all-out-effort to achieve stability of the computation. The objective of the computation is to obtain valid approximations to a given physical problem. In the following review, it is therefore intended to bring out primarily the mathematical assumptions and their physical implications of various approaches when they are applied to the solution of different types of practical problems.

3.1 v. Neumann Stability Analysis

A vector unknown function $U(t,x_j)$ of dimension p is to be calculated over mesh spacings Δx_1 , Δx_2 , Δx_3 for successive increments of Δt from the initial values of $U(t=0,x_j)$ based on a system of linear difference equations.

The general form of the linear difference relation may be that some linear combinations of the values of the function \mathbf{U}^{n+1} at a group of neighboring mesh points are given by some other linear combination of \mathbf{U}^n at various neighboring points. If only the \mathbf{U}^{n+1} evaluated at a single mesh point is involved in the difference equations, the unknown values of \mathbf{U}^{n+1} at any given mesh point can be determined without reference to the advanced values of \mathbf{U}^{n+1} at other mesh points. Such difference equations are explicit. If the advanced values of \mathbf{U}^{n+1} at more than one mesh point

are involved, a set of recursive difference relations written for all the mesh points would have to be solved simultaneously so that the advanced values of all the mesh points in the entire field of computation will be obtained at the same time. Such difference equations are implicit. Sometimes it is preferred to solve simultaneously for the advanced values at special groups of mesh points in succession, such as by rows, by columns, or by diagonals, by blocks or by bands. Such difference equations are partially implicit and partially explicit by nature. The organizations of the special group may change from one to the next, and such different groups are often applied in alternate sequence or in some special orders. They are then referred to as alternating direction methods. The specific details of the difference algorithms that may be employed to represent a differential problem is indeed very numerous.

If all the coefficients of the difference equations are constant, and if the system of equations are to be solved under periodic boundary conditions (or under the presumption that the boundary is so far away as to exert no influence on the solution, i.e., the pure initial value problems), the solution of the system of equations can be extended periodically beyond the field of computation with both U^n and U^{n+1} represented by Fourier series. The linearity of the difference equations system permits the treatment of each Fourier component separately. Thus by substituting U by $V(k_j)$ exp $\{ik_jx_j\}$ into the system of difference equations and cancelling the common factor in each equation, an equation

$$H_1 V^{n+1}(k_j) = H_0 V^n(k_j)$$
 (3.1)

results. Here i is the complex number to represent the sinusoidal functions with wave numbers k_1 , k_2 , k_3 in the x_1 , x_2 , x_3 directions respectively. $V(k_j)$ is the amplitude of the particular wave component under consideration. Each of the Fourier components may be considered either as a part of the proper solution U or as a small perturbation (or error) superposed on the solution U. H_1 and H_0 are the matrix operators depending on the constant coefficients of the difference equations and of Δt and Δx_j . On the assumption that H_1 can be inverted, then Equation (3.1) becomes

$$V^{n+1}(k_j) = G(\Delta t, \Delta x_j, k_j) V^n(k_j)$$
 (3.2)

where

$$G(\Delta t, \Delta x_j, k_j) = (H_1)^{-1} H_0$$

Equation (3.2) tells the evolution of each Fourier component either as a part of the solution or as a perturbing error. Accordingly $G(\Delta t, \Delta x_j, k_j)$ is called the amplification matrix of the system of difference equations. The condition that the solution U should be uniformly bounded requires each and every component to be so bounded. Since the norm of $\|V^{\mathbf{n}}\| \leq \|G\|^{\mathbf{n}} \cdot \|V^{\mathbf{0}}\|$, it is necessary and sufficient that $\|G\|^{\mathbf{n}}$ be so bounded for all wave components and for all $\mathbf{n} = T/\Delta t$ where T is the time period for which U is to be calculated with some choice of small but positive Δt . Now $\|G\|^{\mathbf{n}} \geq \mathbb{R}^{\mathbf{n}}(\Delta t, \Delta x_j, k_j)$ where R is the spectral radius of G, i.e., the largest eigenvalue of G. Hence for such initial periodic boundary value problems, the v. Neumann's condition follows that all the eigenvalues of the amplification matrix G be $\leq 1+O(\Delta t)$. It is a necessary condition for computational stability. The eigenvalues of the amplification matrix are often more conveniently obtained by direct substitution of $\mathbf{u}^{\mathbf{n}+1} = \lambda \mathbf{u}^{\mathbf{n}}$

into the difference equation to obtain the determinant which vanishes when λ takes up the eigenvalues. The v.Neumann condition becomes sufficient for the stability of the stated problem when the matrix G is normal. Both this sufficiency aspect and the additional term $O(\Delta t)$ are without much practical significance for the present consideration as will shortly become clear. The important points to recognize from the above are the physical implications of the various conditions under which the v.Neumann stability analysis is formulated.

3.2 Local Linearization

The application of the v.Neumann analysis for the stability of the numerical integration of a system of nonlinear partial differential equations such as (1.7) calls for quite a few important additional approximations:

- (i) The nonlinear difference (or differential) equation is linearized by considering the solution as the sum of a small perturbation (or variation) superposed over the local solution of the problem. By substituting the perturbed solution into the difference equation and keeping only the terms involving first power of the perturbation, the result is the equation of the first variation with coefficients depending on the solution of the differential problem, such coefficients will vary with x and t.
- (ii) The coefficients, will be assumed to be slowly varying so that these coefficients can be evaluated by the constant local values at various mesh points. The system of equations of the first variation then becomes linear and with constant coefficients for the first variation. It is supposed to apply locally at each mesh point. The coefficients (and hence the difference relations) vary from mesh point to mesh point.
- (iii) The stability behavior of the computation at each mesh point is independent of its neighbors and can be considered as the stability

problem very far away from the boundary (it cannot be periodic). Thus the v.Neumann stability analysis may be applied locally to find the local stability limit on Δt .

(iv) The local stability limit is determined at every mesh point in the interior with the local computed value $U^{n}(x)$ rather than the genuine solution $u(x,n\Delta t)$. The most restrictive of the local stability limits over all the interior points will then be taken as the stability limit on Δt for the integration of the difference problem.

Such a local linear stability analysis to be applied to fluid dynamics problems is probably what led v.Neumann to develop the Fourier method for the constant coefficient linear difference equations. This method is still the most valuable practical tool. It should be noted that slight difference in the linearization procedure can lead to slightly different linearized equations of the first variation. They will give slightly different local linearized stability criteria. Consider the following example:

$$\frac{\partial u}{\partial t} = \frac{\partial^2}{\partial x^2} (u^5) \tag{3.3a}$$

$$= \frac{\partial}{\partial x} \left(5u^4 \frac{\partial u}{\partial x} \right) \tag{3.3b}$$

with the initial condition

$$u_0 = u(x,t=0) = \Psi[v(x_0-x)]$$

and the boundary conditions

$$u(o,t) = \Psi[v(vt+x_o)]$$

$$u(L,t) = \Psi[v(vt-L+x_o)]$$

The following is a solution representing a running wave with constant wave velocity v

$$u(x,t) = Y[v(vt-x+x_0)]$$
 (3.4)

where the function Y is given implicitly as the inverse of

$$\frac{5}{4} (u-u_0)^4 + \frac{20}{3} u_0 (u-u_0)^3 + 15 u_0^2 (u-u_0)^2 + 20 u_0^3 (u-u_0)$$

$$+ 5 u_0^4 \ln(u-u_0) = v(vt-x+x_0)$$
(3.5)

It is shown in Fig. 1 with a relatively sharp front and approximately a quartic curve far downstreams. It may be interesting to note that the Equation (3.3) stands as a heat diffusion equation with variable diffusivity $5u^4$, rather than an equation describing the steady propagation of a nondecaying wave.

Let the Equation (3.3) be discretized with forward time and centered space difference algorithm with the spatial derivative evaluated in part θ at the advanced time step and the other part $(1-\theta)$ at the original time step.

$$U_{j}^{n+1} - U_{j}^{n} = \frac{\Delta t}{\Delta x^{2}} \left\{ \theta \left[\delta^{2} \left(U^{5} \right) \right]_{j}^{n+1} + \left(1 - \theta \right) \left[\delta^{2} \left(U^{5} \right) \right]_{j}^{n} \right\}$$
 (3.6)

where the second order spatial difference operator

$$[\delta^{2}()]_{j}^{n} = ()_{j+1}^{n} - 2()_{j}^{n} + ()_{j-1}^{n}$$
(3.7)

The parameter θ can be chosen at convenience. This is a nonlinear equation. The following linearized approximation

$$(v^5)_{j}^{n+1} - (v^5)_{j}^{n} = 5(v^4)_{j}^{n} (v_{j}^{n+1} - v_{j}^{n})$$

gives the equation of first variation of (3.6) as

$$(\upsilon_{j}^{n+1} - \upsilon_{j}^{n}) - \frac{5\theta\Delta t}{\Delta x^{2}} \left[(\upsilon^{4})_{j+1}^{n} (\upsilon_{j+1}^{n+1} - \upsilon_{j+1}^{n}) - 2(\upsilon^{4})_{j}^{n} (\upsilon_{j}^{n+1} - \upsilon_{j}^{n}) + (\upsilon^{4})_{j-1}^{n} (\upsilon_{j-1}^{n+1} - \upsilon_{j-1}^{n}) \right]$$

$$= \frac{\Delta t}{\Delta x^{2}} \left[(\upsilon^{5})_{j+1}^{n} - 2(\upsilon^{5})_{j}^{n} + (\upsilon^{5})_{j-1}^{n} \right]$$

$$(3.8)$$

Note that the equation is linear in the unknown $(U_j^{n+1}-U_j^n)$ if the values of the function U at all the spatial mesh points at the time level n are known. Otherwise, the equation would have retained its nonlinear form. Alternatively, it is also appropriate to linearize in many other ways. A particularly simple one is to approximate

$$\left[\delta^{2}(U^{5}) \right]_{j}^{n+1} - \left[\delta^{2}(U^{5}) \right]_{j}^{n}$$

$$= 5(U^{4})_{j}^{n} \left[(\delta^{2}U)_{j}^{n+1} - (\delta^{2}U)_{j}^{n} \right]$$
and
$$\left[\delta^{2}(U^{5}) \right]_{j}^{n} = 5(U^{4})_{j}^{n} (\delta^{2}U)_{j}^{n}$$

$$(3.9)$$

Then the equation of the first variation of (3.6) becomes

$$(U_{j}^{n+1} - U_{j}^{n}) - 5 \frac{\theta \Delta t}{\Delta x^{2}} (U^{4})_{j}^{n} \left[(U_{j+1}^{n+1} - U_{j+1}^{n}) - 2(U_{j}^{n+1} - U_{j}^{n}) + (U_{j-1}^{n+1} - U_{j-1}^{n}) \right]$$

$$= 5 \frac{\Delta t}{\Delta x^{2}} (U^{4})_{j}^{n} \left[U_{j+1}^{n} - 2U_{j}^{n} + U_{j-1}^{n} \right]$$
 (3.10)

This last equation is indeed the same as what would result if the effective diffusivity 5u⁴ in Equation (3.3b) should be treated as a constant before and during discretization.

With all U_{j+1}^n , U_j^n , and U_{j-1}^n taken to be constant, the v.Neumann

stability analysis for Equation (3.8) will require the following absolute value to be less than unity for all wave number k.

$$\left| \begin{array}{c|c} \frac{1 - (1 - \theta)s}{1 + \theta s} \right| \leq 1 \tag{3.11}$$

where s is the complex expression

$$\mathbf{s} = \mathbf{5} (\mathbf{U}^4)_{\mathbf{j}}^{\mathbf{n}} \frac{\Delta \mathbf{t}}{\Delta \mathbf{x}^2} \left[2 - (\alpha + \beta) \cos k\Delta \mathbf{x} - i(\alpha - \beta) \sin k\Delta \mathbf{x} \right]$$
with $\alpha = (\mathbf{U}_{\mathbf{j}+1}^{\mathbf{n}}/\mathbf{U}_{\mathbf{j}}^{\mathbf{n}})^4$
and $\beta = (\mathbf{U}_{\mathbf{j}-1}^{\mathbf{n}}/\mathbf{U}_{\mathbf{j}}^{\mathbf{n}})^4$

The restriction on the value of $\frac{\Delta t}{\Delta x^2}$ can be computed for all k from (3.11) for different values of α and β at every interior mesh point. This is a very tedious process. The v.Neumann stability analysis for Equation (3.10) leads to the same relation (3.11) but with $\alpha=\beta=1$. This provides an explicit limit on $\frac{\Delta t}{\Delta x^2}$ that when $\theta < 1/2$,

$$5(U^4)_j^n \cdot \frac{\Delta t}{\Delta x^2} \le \frac{1}{2(1-2\theta)}$$
 (3.12)

and there will be no limit on $\frac{\Delta t}{\Delta x^2}$ if $\theta \ge 1/2$. This is the well-known results for the simple heat equation.

To test the usefulness of the local linear stability criterion, computations were carried out at θ = 0.4 and $\frac{\Delta t}{\Delta x^2}$ = 0.001 with Equation (3.8). The parameters v and U were chosen as $v\frac{\Delta t}{\Delta x}$ = 0.075 and $5U_0^4 \frac{\Delta t}{\Delta x^2}$ = 0.005. The last value is much less than 2.50 as is required by Equation (3.12) for local computational stability. As the computation proceeds, the values of U increases with to entire field of computation. According to the local stability criterion (3.12), we would expect instability to appear in the form of rapidly increasing amplitudes of oscillations when

and where the values of $(U_j^n)_0$ exceed $(500)^{1/4} \sim 4.7$. This was what happened as is illustrated in Fig. (1). The computed points lie very close to the analytical solution except at the foot of each wave front where the solution undergoes a rapid change and in the region where $U_j^n/U_0 > 5$ and where the computed solution oscillates, signalling the onset of computational instability.

It is remarkable that the simple local criterion deduced for the difference Equation (3.10) provides highly satisfactory guidance for the integration of Equation (3.8) although α and β generally differ from unity. Where the stability boundary of Equation (3.8) with $\alpha \in \beta \neq 1$ lies within the stable region of Equation (3.10), the local linear stability limit need not even be "necessary" at such interior points. Such regions are likely to be small, however, if the model equation (3.10) in the above example is appropriately chosen. It is clearly not sufficient since the v.Neumann stability condition itself is not and since the influence of the boundary conditions on computational stability is yet to be investigated. Nevertheless, the local linear stability analysis does appear to provide useful guidance in practical applications especially if the influence of the boundary conditions can be separately investigated and if the linearized model for the difference relations at the interior points are properly selected. Such fortunate circumstances are, however, not to be presumed in complicated equations systems.

3.3 Application to Navier Stokes Equations

The Navier-Stokes equations system is quasi-linear due to, (i) the variable convective velocity, (ii) the variable density and energy and hence the variable diffusivity as illustrated in Equation (3.3). It is

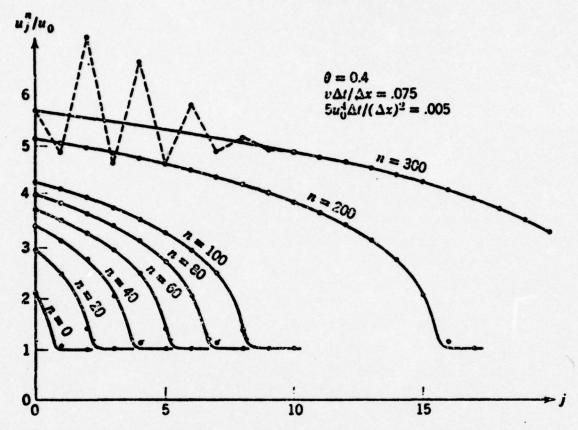


Fig. 1. Running-wave solutions of the non-linear equation $\partial u/\partial t = \partial^2(u^6)/\partial x^2$. The curves show the exact solution, given by equation (8.25) and the dots show the solution of the difference equation (8.27) with $\theta = 0.4$ and with Δt and Δx so chosen that $v\Delta t/\Delta x = 0.075$ and $5u_0^4\Delta t/(\Delta x)^2 = 0.005$. The numbers on the curves are cycle numbers.

further complicated by the small diffusivity or large Reynolds number and the presence of many such terms especially in multi-dimensional flow problems. If the standard procedure of local linearization is followed, the resulting linearized equations are very long. The v.Neumann stability analysis for such equations will inevitably lead to unwieldy algebraic expressions so that the explicit limit on Δt at each mesh point can only be obtained at much more labor than what is required in the situation of Equation (3.11). It is impractical to consider checking the stability limit at many mesh points even if infrequently. It appears imperative to look for simple but meaningful model equations such as Equation (3.10) in the previous example. This is considerably complicated by the change of the asymptotic behavior of the Navier-Stokes equations system in different regions in the field of computation, enumerated in the previous chapter. Near the solid boundaries or where the viscous effects are important, the region is locally parabolic or elliptic. Far away from the solid boundaries, the direct viscous effect is negligible and the flow region is primarily hyperbolic. It is unfortunate that a difference algorithm, when applied to practical differential equations of different types, will lead to difference equations with quite different stability behavior.

Tables I and II list a few common difference algorithms when applied to the simple wave equation and to the simple diffusion equation respectively. An algorithm often yields a stable difference equation for the diffusion equation such as the forward time-centered space algorithm (Scheme 1 in Table II) while it provides an unstable difference equation (Scheme 3 in Table I) from the simple wave equation. Friedrichs modification, which renders the wave problem stable (Scheme 4 in Table 1), on the other hand, leads to an unstable diffusion problem (Scheme 2 in

Table II). The centered time and centered space algorithm is another example which is given in these tables. There are many other examples like these. Such schemes are therefore not useful for integrating Navier-Stokes equations.

There are many other schemes which are stable for both types of equations but Δt are subject to different restrictions in different regions. Usually $c\frac{\Delta t}{\Delta x} < 1$ for the wave equation and $\frac{\Delta t}{\Delta x^2} \leq$ some fractional constant g for the diffusion equation; such as the forward time, backward space, Scheme 1 and 2 respectively in the two tables. The condition $c\frac{\Delta t}{\Delta x} \leq 1$ is known as the Courant-Friedrich-Levy (CFL) condition of zone of dependence to be satisfied generally for difference forms for wave equations. [1] It states that the zone of dependence of the differential equation. When such a scheme is used in integrating the Navier-Stokes equations, computational stability might be expected if Δt is locally chosen to be the more restrictive of the diffusion limit and of the wave limit: [2]

$$\Delta t < Inf \left[\frac{\Delta x}{c}, \gamma \frac{\Delta x^2}{v} \right]$$
 (3.12)

where c is related to the local wave speed, ν is the local kinematic viscosity coefficient, and γ is some constant less than unity. The precise values of c and γ may be determined from the ν . Neumann stability analysis of the linearized Navier-Stokes equations after dropping the viscous terms or the dynamic terms respectively. The most restrictive of these local limits over all the mesh points may then be taken as the Δt for the next time increment. In actual computations, it is often necessary to reduce this most restrictive limit on Δt further by introducing an empirical safety factor which may have to be rather small.

Some safety factor may have to be needed because of the unknown effect of the boundary conditions. But actual computation often indicates the instability to be initiated from the interior. Thus, it appears to be, at least in part, due to the fact that the pure diffusion and/or the pure wave equation are rather poor models for the interior points of the linearized Navier-Stokes equations. It is true that in the linearized form the Navier-Stokes equations may be visualized as the superposition of a wave and a diffusion equation. The stability limit is, however, not generally the superposed diffusion and the wave limit. This is because the determination of the eigen-values of a linear equation is not a linear problem, which requires the solution for the roots of a polynomial equation with constant coefficients. A small perturbation on a coefficient of the characteristic polynomial often leads to an inproportionately large change in the largest eigenvalue (or the spectral radius) depending on the specific difference algorithm.

To illustrate the situation, consider the one-dimensional Burgers' equation with constant c and v.

$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = v \frac{\partial^2 u}{\partial x^2}$$
 (3.13)

When c and V are taken as the local values at a mesh point, it serves as a linearized model of the Navier-Stokes equation in one space dimension, with the essential characteristics of changing type of the partial differential equation. If Equation (3.13) is discretized with forward time backward space difference for the convective term and the centered space difference for the diffusion term, the v.Neumann stability limit is

$$\Delta t \leq \left(c/\Delta x + 2v/\Delta x^2 \right)^{-1} \tag{3.14}$$

which is almost half of the hyperbolic limit $\Delta x/c$ or the diffusion limit $\Delta x^2/2\nu$ if they are approximately equal. Thus the safety factor to be applied to the condition (3.12) should be about 1/2 or less for the stable computation of the interior points alone.

The situation is even more critical for multidimensional flow problems. Consider the two different models for 2-D problems

$$\frac{\partial u}{\partial t} + c \left(\frac{\partial u}{\partial x} + \frac{\partial u}{\partial y} \right) = v \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$
and
$$\frac{\partial u}{\partial t} + c \frac{\partial u}{\partial x} = v \left(\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} \right)$$
(3.15)

with the convective term $v \frac{\partial u}{\partial y}$ in the dynamic terms represented by $c \frac{\partial u}{\partial y}$ and zero respectively. The stability limits for the two cases assuming $\Delta x = \Delta y$ are

$$\Delta t \leq \frac{1}{2} \left(c/\Delta x + 2v/\Delta x^2 \right)^{-1}$$
and
$$\Delta t \leq \left(c/\Delta x + 4v/\Delta x^2 \right)^{-1}$$
(3.16)

respectively. This means that the safety factor to be applied to condition (3.12) should be ~1/4 and 1/3 for 2D flow problems and even smaller for the 3D flow problems. Thus, the stability condition (3.12), based on superposing the wave and the diffusion parts of the Navier-Stokes is not very useful although it is simple and convenient.

The local stability condition based on the linearized Burgers' equation was found to be quite satisfactory for the integration not only of the nonlinear Burgers' equation without a safety factor, but of the full Navier-Stokes equations when the boundary conditions are properly treated. The one-dimensional Burgers' model should be applied locally

to the flow along the streamline through a mesh point. This will yield stability limits of the form of Equation (3.14) and (3.16) in which c should be interpreted as the local signal speed |q| + |a|. Here q is the stream velocity. Both the local speed of sound a and the kinematic viscosity coefficient v should be evaluated at the local temperature or energy. Ax should be evaluated along the streamline in some manner and may well be taken as the smaller of $(\Delta x , \Delta y)$ for 2-D problems for example. The different details how these local quantities may be approximated by those explicitly calculated at each point, will give large varieties of expressions for evaluating the local stability limit on Δt for a given choice of the difference algorithm for discretization. It is advisable to choose a simple form convenient for the explicit determination of the limit on At at each point, although less accurate. This calculation is to be carried out at many points and at many time intervals for an estimate of the most restrictive limit (the smallest value of) on Δt for the next time interval. It may also be convenient to check the local linearized stability limit once every few time steps rather than at everytime step and to adjust the magnitude of Δt adopted in the computation for the next few steps accordingly.

3.4 Treatment on the Boundary

When the appropriate local linearized stability limit is obeyed, computational instability at the interior points can usually be avoided although oscillations of fairly large but bounded amplitudes are often present in the calculated results. These oscillations originate from the boundaries, both interior and exterior and do not represent computational instability in the sense of boundedness of the solution discussed

previously. Such bounded oscillations are often referred to as the Nonlinear Instability which is basically a different phenomenon more directly related to the question of accuracy and can doubtfully be clarified by the heuristic local linear stability treatment discussed in the previous section.

Genuine unstable computations can result when certain boundary treatment is applied to some difference algorithm. For such cases, the local linearized analysis can often tell the impending computational instability. Consider the integration of the inviscid gas dynamic equation (2.7) with the Leap-Frog scheme, (Scheme 5 in Table I)

$$U_{j}^{n+1} - U_{j}^{n-1} = -A_{j} \frac{\Delta t}{\Delta x} \left[U_{j+1}^{n} - U_{j-1}^{n} \right]$$
 (3.17)

which is second order accurate in both time and space and is always stable for any values of $\Delta t/\Delta x$ at all the interior points. To initiate the integration, both U_j^0 and U_j^1 should be available at all j=0,1,2,...J and boundary conditions must be provided at both boundaries j=0 and j=J. Note that both the initial value U_j^1 and the boundary data at j=J are not specified by the initial data of the differential problem of the propagation of a small wave in an unbounded flow field. These data are extraneous and are brought about by the use of the higher order accurate difference algorithm in which a first order differential coefficient is replaced by a second order difference quotient.

The extraneous initial data U_j^1 are usually obtained from U_j^0 and the temporal derivatives through Taylor series about t=0. The higher order temporal derivatives are obtained from the initial data U_j^0 in the vicinity

of the point based on the differential relation and its time derivatives. It is not obvious how the extraneous boundary data at j=J should be defined. One of the natural ways is to extrapolate along x assuming that $\frac{\partial}{\partial x}$ U is small is

$$U_{J}^{n} = U_{J-1}^{n} (3.18)$$

This is not a bad physical approximation. Computationally it leads to the difference relation

$$U_{J-1}^{n+1} - U_{J-1}^{n-1} = -A_{J-1} \frac{\Delta t}{\Delta x} \left[U_{J-1}^{n} - U_{J-2}^{n} \right]$$
 (3.19)

for advancing the mesh value at J-1 immediately preceding the boundary point J. If the v.Neumann stability analysis is applied locally to this difference equation with A_{J-1} taken as a constant, and U taken as a scalar unknown, this difference relation (3.19) is locally always unstable with the amplification factor $|\lambda| = |U_{J-1}^{n+1}/U_{J-1}^{n}| > 1$. This is because the v.Neumann analysis leads to the algebraic relation

$$\lambda - \frac{1}{\lambda} = -A_{J-1} \frac{\Delta t}{\Delta x} \left[(1 - \cos k\Delta x) + i \sin k\Delta x \right] = -2(f_r + if_i)$$
 (3.20)

where k is the wave number under consideration and 2f, and 2f, are the real and the imaginary parts of the right hand side. Thus

$$\lambda = -(f_{r} + if_{i}) \pm \left[1 + (f_{r} + if_{i})^{2}\right]^{1/2}$$
 (3.21)

For some choice of k, f_i will be zero and the absolute value $|\lambda|$ will be greater than unity regardless of the magnitudes of $A_{J-1} \frac{\Delta t}{\Delta x}$. Actual computation confirms the instability that $|U_J^n|$ diverges as n. If $A_{J-1} \frac{\Delta t}{\Delta x}$ should be taken as unity and if the initial data satisfies $U_J^n = (-1)^{j+n}$

for n = 0 and 1 and all j = 0, 1...J-1, the solution of the difference equation actually can be shown to continue as

$$U_j^n = (-1)^{j+n} + (-1)^j F(j+n)$$

with
$$F(j + n < J) = 0$$
 and $F(n + J) = (-1)^{n-1}2n$ (3.22)

Higher order accurate extrapolation formulas based on zero higher order derivatives instead of Equation (3.18) will only change f_r and f_i and still lead to computational instability in the same manner.

Careful examination of the local stability analysis will suggest that stable computation will result if the extraneous boundary value $\mathbf{U}_{\mathbf{I}}^{\mathbf{n}}$ is obtained as:

$$U_{J}^{n} = \frac{1}{2} \left(U_{J-1}^{n+1} + U_{J-1}^{n-1} \right)$$
 (3.23)

i.e., U_{J-1}^{n} in the first order extrapolation formula (3.18) is replaced by the average of its temporal neighbors. Then the difference relation on the boundary is

$$U_{J-1}^{n+1} = \frac{1-\alpha}{1+\alpha} U_{J-1}^{n-1} + \frac{2\alpha}{1+\alpha} U_{J-2}^{n}$$
 (3.24)

where $\alpha = \frac{1}{2} A_{J-1} \frac{\Delta t}{\Delta x}$ with $\alpha > 0$.

$$|U_{J-1}^{n+1}| \leq \max (|U_{J-1}^{n-1}|, |U_{J-2}^{n}|)$$
 (3.25)

and the advanced values U_{J-1}^{n+1} remains bounded. Alternatively if the v.Neumann analysis is followed, then

$$\lambda = \frac{1-\alpha}{1+\alpha} \frac{1}{\lambda} + \frac{2\alpha}{1+\alpha} e^{-ik\Delta x}$$
and
$$|\lambda| \le \left| \frac{1-\alpha}{1+\alpha} \right| \frac{1}{|\lambda|} + \frac{2\alpha}{1+\alpha}$$
Thus
$$-1 < -\frac{1-\alpha}{1+\alpha} < |\lambda| < 1 \quad \text{if } \alpha < 1$$
or
$$-1 < |\lambda| < \frac{\alpha-1}{\alpha+1} < 1 \quad \text{if } \alpha > 1$$

and computational stability can be expected.

Thus the local linear stability analysis will help to avoid unfortunate choices of the unstable boundary conditions and sometimes suggest appropriate choices to secure stable computation. It must be cautioned that if the particular choice of the boundary condition fails to represent the physical situation, the computed stable solutions need not be a good approximation to the solution of the physical problem. It is common that oscillations of finite amplitudes appear to be generated at the various boundaries in a computed stable solution and that such oscillations appear to propagate into the interior of the field of computation, (or away from the shock wave or other interior boundaries). They represent oscillatory error components, superposed on the correct solution of the physical problem and are likely introduced by the "errors" in the difference treatments of such boundaries. Indeed there are also nonoscillatory errors caused by the difference treatments on the boundary and such errors may actually be more serious because of its deceptively smooth appearance in the results of a stable computation. Such errors tend to be overlooked especially in view of the difficulties in securing a stable computation. An important aspect of studying the accuracy of the computed results is to recognize if the various boundary conditions are appropriate and to estimate the associated errors.

IV. IMPLICIT COMPUTATION AND RATE OF CONVERGENCE

Implicit difference algorithms generally lead to stable difference equations when applied to simple wave and simple diffusion equations as is indicated in Tables I and II. The local linear stability analysis for equation (3.3) illustrates further that stability is "improved" when the fraction θ of the spatial derivative evaluated at the advanced time level (and hence implicit) is increased from zero to 1/2. The system becomes unconditionally stable when $\theta \geq 1/2$. The implicit difference algorithms are traditionally used in the solution of Laplace or Poisson equations without any problem of computational stability. The implicit difference algorithm then appears to be the most desirable from the point of view of avoiding computational stability especially for complicated problems with mixed behavior. It will be demonstrated that the merit of the implicit schemes is not really that obvious. There are indeed other difficulties which may be more serious than computational stability.

In implicit difference algorithms, the difference relation at a given mesh point contains the unknown advanced values of quantities at it neighboring mesh points. It is necessary to treat the system of difference relations at all the interior mesh points simultaneously to solve for all the unknowns at all the interior mesh points. Thus the difference formulation based on a totally implicit scheme will require the inversion of matrices of vary large dimensions. This imposes severe requirements on the memory capacity and on the arithmetic speed of the computer. This also calls for skills in rendering efficient inversion of the sparse but large matrices and inevitably through some form of iterative procedures.

The rate of convergence or the number of iterations required to solve the system of equations to a prescribed accuracy is of great concern. This is because the computational effort required to complete a "sweep" over the field of computation (i.e. to advance the values of the functions at all the mesh points for one time step) is generally much larger for the implicit difference formulation than for the explicit difference formulation. It is hoped, however, that, in the absence of a stability limit on Δt with the implicit difference formulation, the time steps may be taken so many times larger than the time step allowed by the stability limit of the explicit formulation as to more than compensate for the much larger computational effort per time step for the implicit formulation. In the following sections this question will be examined.

4.1. Simple Time Dependent Problem.

The advantage of the implicit formulation is best illustrated in the solution of the time dependent heat transfer problems in multispace dimension or in the solution of Laplace equations for the steady state problem.

$$\frac{\partial u}{\partial t} = v\nabla^2 u \tag{4.1}$$

For such problems, the system of simultaneous difference equations to be solved can be conveniently arranged to be

$$AU = f \tag{4.2}$$

where U is the vector unknown representing the temperature at all the N interior mesh points, arranged in some appropriate order. f is a known vector of dimension N and A is an N x N tridiagonal matrix often diagonally dominant. The solution of the system (4.2) for the unknown vector U is

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The mathematical foundation and the various practical aspects of the numerical solution of gas dynamic equations are critically reviewed with emphasis on obtaining quantitatively accurate solutions for application in various engineering and sciences Computational stability rate of convergence and accuracy (or error estimate) are discussed. The promises and problems of the 4th generation computers are outlined within this perspective.)

Computational stability should not be obtained at the sacrifice of the convergence rate to and the accuracy of the final solution. With accuracy in mind, the explicit algorithms are likely preferrable to the implicit ones. Strict conservation of the difference formulation is recommended and exemplified to avoid the accumulation of local truncation errors and to facilitate the estimate of the errors in a steady state solution. Illustrative examples are given including supersonic flows with shocks.

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equivalent to the inversion of the matrix A, giving U as $U = A^{-1}f$. Computationally, a highly efficient method can be used to solve the system (4.2) with approximately 5N operation counts. (Conventionally, each multiplication and division counts as one operation while addition, substraction and other data management operations are neglected). This is to be compared with N counts for the solution of an explicit system. (The evaluation of coefficients is ignored here on the presumption that the same amount of computational work is needed in both the implicit and the explicit cases). Thus the computational effort to advance the solution for one time step with the implicit format is about 5 times as much as that with an explicit format. As is illustrated in Table 2, most stable explicit schemes will possess the stability limit (easily verified by v. Neumann analysis) of the type s = $\frac{v\Delta t}{\Delta r^2}$ < (1/2, 1/4); here 1/4 is for two dimensional problems (see equation 3.16 with c = o.). With good spatial resolution, i.e. a small Ax, the time step for the explicit scheme will be limited to $\Delta t \lesssim \frac{1}{2\nu} \Delta x^2$ which is indeed very small. Thus, if computations with the implicit formulation should be carried out with a time step larger than $\frac{5}{2V}\Delta x^2$ or even taken as $\Delta t = \Delta x$, considerable saving in the computational effort results in the determination of the temperature field V at that later time.

The benefit that results is, however, illusory if the determination of the solution at some specific later time is required to possess a specific accuracy. Suppose that all the variables are properly non-dimensionalized and that it is required to achieve an accuracy of 10⁻², assumed to be solely dependent on the truncation error (i.e. all the other errors are suppressed in the formulation and computation). Then if the explicit algorithm 1 in

table II is used, which is first order accurate in time and second order accurate in space (i.e. $e_t = 0(\Delta t, \Delta x^2)$, the field of computation defined by x = 0 to 1 and y = 0 to 1 for a two dimensional problem from time t = 0 to 1 should be divided into at least 10 equal parts in both the x and the y direction, i.e. $\Delta x = \Delta y = 1/10$, preferably say with $\Delta x = \Delta y = 1/20$ to allow some margin of safety. The stability limit will require a Δt (with time non-dimensionalized by the square of characteristic length divided by the diffusivity) as small as $\frac{1}{4} \Delta x^2 = 10^{-3}$ if $\Delta x = 1/20$ or $1/4 \times 10^{-2}$ if $\Delta x = 10^{-1}$. The relative magnitudes of Δt and Δx are such that the local truncation error $e_t = 0(\Delta t, \Delta x^2)$ and hopefully the computed results will remain consistent with the accuracy requirement. (In this case, the accumulation of the local truncation error will remain of the same order.)

If now, the scheme (1) in Table II is modified so that the spatial derivative is replaced by the implicit difference

$$v_{j+1}^{n+1} - 2v_{j}^{n+1} + v_{j-1}^{n+1}$$
)

for both x and y direction with the same local truncation error $e_t = 0(\Delta t, \Delta x^2)$. This scheme (Lassonen) is unconditionally stable, i.e. Δt can be taken arbitrarily large compared with Δx without suffering computational instability. However, with Δt much larger than Δx^2 , the local truncation error is of $0(\Delta t) \gg 0(\Delta x^2)$. Thus with $\Delta x = 1/20$ as was in the explicit case and if Δt is taken as $\Delta x/5$, which is 16 times larger than the stability limit of the explicit scheme, the computational effort will be only $\sim 1/3$ of that with the explicit scheme. The solution so obtained is; however, less accurate with $e_t = 0(\Delta t)$ and $\Delta t = \frac{\Delta x}{5} = 10^{-2}$, marginally acceptable to the required accuracy 10^{-2} , allowing no room for the accumulation of the local truncation errors. Formally, this solution from the implicit scheme

should be compared with the solution from the explicit scheme with $\Delta x = 10^{-1}$ with $e_t = 0(\Delta x^2)$ and $\Delta x^2 = 10^{-2}$. The computational effort of this explicit scheme is actually only 80% of the implicit scheme with the same local truncation error. Alternatively if the implicit scheme is to produce a result with accuracy comparable to the explicit solution computed with $\Delta x = 1/20$ and $\Delta t = 1/4 \times (\frac{1}{20})^2$. The time step Δt for the implicit calculation should be taken at most as $\Delta x^2 = \frac{1}{400}$ so that $e_t = 0(\Delta t = \Delta x^2)$. Then the computational effort for the explicit format will again be 80% of that of the implicit format of comparable accuracy.

The effectiveness of the implicit algorithm is largely nullified by the first order temporal accuracy of the difference scheme in the above example. It may be that implicit schemes with second order temporal accuracy will be more effective in reducing the overall computational effort, but such higher order schemes will be cumbersome. From this point of view alone, the implicit schemes would appear to be certainly advantageous in the solution of steady state problems via asymptotic temporal approach since the temporal accuracy is of little concern But, as will be discussed in the naxt section, it is not certain if the large temporal steps is conducive to rapid convergence to the steady state. It should be noted in the above example, that the solution of the implicit formulation calls only for the inversion of a tridiagonal matrix which can be implemented most efficiently in ~ 5N operations. For fluid dynamics problems, the matrices resulting from an implicit formulation will be far more complex and the solution of such matrix equations will be far more time consuming. It appears prudent not to expect significant savings in the computational effort by the use of implicit difference algorithms without some detailed investigation.

4.2 Iterative Solution of Steady State and Asymptotic Temporal Approach

Most of the fluid flow problems of practical interest are at steady state or quasi-steady state in which the temporal variations of the flow variables are negligible. Discretization of such steady state equations will generally lead to implicit difference relations in terms of the steady state values of various physical quantities at all the interior points and the boundary values. Except for the solution of potential flow problems of incompressible fluids, the differential equations will be non-linear and considerably more complicated than the Laplace equation. The resulting implicit difference relations will give rise to a rather sperse matrix A, when written in the format of equation (4.2). The sparse matrix A will not be tridiagonal or block-tridiagonal, or other spcial forms convenient for the solution of the system of equations. In fact the nonlinear terms will first have to be quasi-linearized so that the coefficients in matrix A can be evaluated with some assumed approximate values. The system of linear equations will then be solved iteratively until the solution from (4.2) agrees with the assumed solution under certain convergence criteria.

Let superscript n indicate quantities evaluated with the nth iterate of U and use the system of difference relations (4.2) to calculate the (n+1)th iterate. Then equation (4.2) becomes

$$A^{n}v^{n+1} - f^{n} = 0 (4.3a)$$

which is indeed the same as

$$A^{n}(U^{n+1}-U^{n}) = f^{n} - A^{n}U^{n}$$
 (4.3b)

Equation (4.3b) can now be considered as obtained from a time dependent equation in which terms with spatial derivatives are the same as those in the steady state equation (4.2) but with an added temporal term

$$\Delta t + o \Delta t A^n \frac{v^{n+1} - v^n}{\Delta t} \stackrel{?}{=} \Delta t A(u) \frac{\partial u}{\partial t}$$

with forward temporal difference quotient replacing $\frac{\partial u}{\partial t}$.

The iterative solution of a steady state problem based on an implicit algorithm then is not substantially different from the solution of a time dependent problem, albeit the artificial temporal term may not correspond to the temporal terms in the time dependent form of the Navier-Stokes equations. The physical meaning of the individual fictitious temporal terms can be easily identified when the matrix operator A is written in expanded form. Thus the iterative index n can be identified with the temporal index n in the time dependent formulation although the equivalent time dependent physical problem may contain artificial sources of mass, momentum and energy. These artificial sources are small but distributed over the entire field of computation, in the interior as well as on the boundary, and vanish in the steady state limit.

In the numerical solution of the Navier-Stokes equations in multispace dimensions, there will be a few thousand mesh points and 4 or 5 unknown quantities at each mesh point. The dimension N of the vector U is commonly $O(10^4)$ or larger. To solve equation (4.3a) for the successive approximations to the solution of the nonlinear equation (4.2) at each time or iterative step by the standard Gaussian elimination process, requiring $\sim \frac{1}{3} \, \mathrm{N}^3$ operations per step, is out of the question. It is imperative to develop highly efficient iterative methods. Thus in equations

(4.3), the matrix operator A^n is split into two parts with B^n operating on U^{n+1} and (A^n-B^n) operating on U^n . Thus

$$E^n U^{n+1} + (A^n - B^n) U^n = f^n$$
 (4.4a)

or

$$B^{n}(U^{n+1} - U^{n}) = f^{n} - A^{n}U^{n}$$
 (4.4b)

where B^n may be some conveniently invertible matrix so that U^{n+1} can be conveniently solved. This U^{n+1} will replace U^n in the next iteration until finally $U^{n+1} = U^n$ according to some steady state criterion. In this manner, the iterative solution of the quasi-linearized equation (4.3) has incorporated the iterations that were called for by the quasi-linearization of the nonlinear equation.

If B is chosen as the identity matrix L equation (4.4b) becomes identical with the difference equation obtained from the explicit scheme, using the forward time difference algorithm and the spatial difference algorithm of the implicit equation (4.3a). Thus, like the solution of time dependent equations with explicit schemes, the iterative solution of equation (4.4b) with B = I corresponds to tracing the physical development of the time dependent flow field from an initial state toward the steady state. The local accumulations of mass, momentum and energy in the cell around each mesh point are precisely how they would be expressed in the explicit scheme for the time dependent flows.

The matrix B may be chosen to be diagonal with its diagonal elements equal to the diagonal elements of A, i.e. $b_{ii} = a_{ii}$ and $b_{ij} = 0$ for $i \neq j$. Such an iterative process is known as Jacobi iteration. Since $b_{ii} = a_{ii}$ are not identically unity, the temporal terms may be larger (or smaller)

than the accumulation term in the physical, time dependent flow. The excess (or deficiency) of that particular quantity U may be attributed to the presence of a source (or sink) of that quantity at the mesh point under consideration. These artificial sources (sinks) will tend to zero when the asymptotic steady state is approached.

If the matrix B is chosen to be the main tridiagonal elements of A, i.e. $b_{ij} = a_{ij}$ for $|i-j| \le 1$ and $b_{ij} = 0$ for |i-j| > 1; then the artificial temporal terms will contain spatial derivatives. They represent the doublets and quadruples of the source-sink pairs around the mesh point. The situation is quite complicated algebraicially and physically, but it is very natural physically how a steady state may be reached via such time dependent states provided that all these sources and doublets etc. properly vanish in the steady state limit. In practice the choice of B is dictated by the desire to reduce the computational effort in obtaining the steady solution, irrespective of its physical correspondence to some temporal flow field. The purpose here is to show that the asymptotic temporal approach and the iterative solution of the implicit formulation to obtain steady state results are fundamentally similar. The iterative method does take much larger computational effort per iteration or per time step. But it permits the use of a much wider variety of temporal artifices to produce a very rapid convergence to the steady state, possibly with less overall computational effort. It is possible, of course, that for some choices of B, there may not be any steady state solutions or there may be steady state solutions different from what is desired as the corresponding physical situation may suggest.

4.3 Iterative Methods

One of the most popular choices of B is the lower triangular matrix part of A i.e. $b_{jk} = 0$ if k > j and $b_{jk} = a_{jk}$ if $k \le j$. This is the Gauss-Seidel iteration or successive relaxation procedure. The $(n+1)^{th}$ iterate is given as

$$v_{j}^{n+1} = \frac{1}{a_{jj}^{n}} \left(f_{j}^{n} - \sum_{k=1}^{j-1} a_{jk}^{n} v_{k}^{n+1} - \sum_{k=j+1}^{N} a_{jk}^{n} v_{k}^{n} \right)$$
 (4.5a)

from which the successive scalar components of Uⁿ⁺¹ can be emplicitly calculated in the order of increasing j in which the latest available mesh values are used throughout. This semi-explicit solution of Uⁿ⁺¹ can be given in matrix form as:

$$U^{n+1} = U^n + (B^n)^{-1} (f^n - A^n U^n)$$
 (4.5b)

Here $(f^n-A^nu^n)$ is the residue and $(B^n)^{-1}$ is the inverse of the matrix B^n .

If the vector calculated from equations (4.5) is taken as a provisional solution and if the new iterate U^{n+1} is evaluated as some weighted average of U^n and this provisional value with weights (1- β) and β respectively, then,

$$\mathbf{U}^{n+1} = (1-\beta) \mathbf{U}^{n} + \beta [\mathbf{U}^{n} + (\mathbf{B}^{n})^{-1} (\mathbf{f}^{n} - \mathbf{A}^{n} \mathbf{U}^{n})]$$
 (4.6a)

which is the same as

$$u^{n+1} = u^n + \beta(B^n)^{-1} (f^n - A^n u^n)$$
 (4.6b)

or =
$$U^n + (B^n/\beta)^{-1} (f^n - A^n U^n)$$

The β is often called the acceleration or relaxation parameter. Equation (4.6b) suggests that β may be interpreted alternatively as a multiplier of the

residue in equation (4.5) or of the operator B^n of the artificial temporal sources in equation (4.4b). The purpose is to effect a faster convergence of the iterative sequence by choosing an appropriate value of β . This process is referred to as successive over (or under) relaxation when $\beta > 1$ (or $\beta < 1$). For the integration of Laplace equation in a rectangular domain, the optimal relaxation parameter β^* for the fastest convergence can be evaluated from the mesh spacing and is usually around 1.8-1.5. For more complicated situations, the choice will have to be empirical and the optimal choice need not even be an over-relaxation. Unfortunate choices of β could lead to diverging sequences, even for Laplace equation (i.e. beyond $2 \ge \beta \ge 0$).

Each Gauss-Seidel iterative step requires N^2 operations. This is to be compared with the counts of $N^3/3$ for Gauss elimination solution for the quasi-linear steady state. The iterative solution would be advantageous if it converges within N/3 iterations since the nonlinear iterations for the solution of equation (4.3) would then be avoided. Now with $N = 0(10^3)$, it is hoped that by proper choice of the relaxation parameter β , much fewer iterations than N/3 may be needed to reach a steady state. In principle, if the steady state is defined by $||U^{n+1}-U^n||/||U^n||| < 10^{-m}$, the number of iterative steps required to converge can be estimated by M/R where R is the rate of convergence with $R \stackrel{\sim}{=} \log_{10}(\frac{1}{\rho})$ and ρ is the geometric mean of the spectral radii of the matrices $(\beta^n)^{-1}$ A^n at successive iterative steps n. Such an estimate of R is not possible in practice because of the complexities of the matrix A and its dependence on the solution U^n .

For the integration of some form of hydrodynamic equations, it is not uncommon that hundreds of such iterations were needed. This is partly due to the nonlinearity of the equations system and partly due to non-optimal choices of the relaxation parameter. It is also often that such iterations fail to converge despite wide range of choices of the acceleration parameter. Now, if the physical state of the flow is steady or quasi-steady, the asymptotic temporal approach of using the correct time dependent equations (B-I) may be expected to converge on purely intuitive grounds, provided that the difference system is stable and consistent with the time-dependent Navier-Stokes equations. But when the implicit iterative mathod is used, its convergence to the steady state cannot be presumed on physical grounds. The artificial sources of mass, momentum and energy are introduced purely algebraically. The particular temporal variations of these sources need not provide any steady state, although without such external artificial sources, nature has demonstrated that a steady state will eventually be reached. It might even be legitimate to question if the steady state so reached should be the same as the one reached under zero external sources since the time integrals of the artificial sources may have altered appreciably the integrals of motion of the system. It is regrettable that no useful answer can be derived physically.

Mathematically speaking, the matrix B in equation (4.4b) can be quite arbitrary and chosen in a great many different ways and even be chosen differently for different steps. Convergence to steady state is assured provided that

$$\lim_{n\to\infty} (B^n)^{-1} (B^{n-1})^{-1} (B^{n-2})^{-1} \dots (B^1)^{-1} (B^0)^{-1} = 0$$
 (4.7a)

and
$$\lim_{n\to\infty} [(B^n)^{-1}A^n][(B^{n-1})^{-1}A^{n-1})] \dots [(B^n)^{-1}(A^n)] = 0$$
 (4.7b)

They can be secured if the spectral radii of all (Bⁿ) -1 and (Bⁿ) -1 Aⁿ are less than unity. If the form of B chosen should be the same for all iterations, (4.7b) is not really much different from the local linearized stability criterion of v. Neumann with the amplification matrix G replacing B⁻¹A. (See Chapter III, Section 3.1 and 3.2). The essential difference lies then in the freedom of choices of the form of the matrices Bⁿ, at different iterative steps n. It is not clear if the condition (4.7a) would imply the physical requirement of the conservation of the integrals of motion. It is also not practical to find the spectral radii or bounds of the eigen values of these complicated matrices. There is no counterpart of the local, linear stability smalysis to provide some idea of the rate of convergence of a complicated problem. There is only the practical solution of trying it out on the computer.

In practice, the possible choices of the form of B is severely limited by its being easily invertible to facilitate the computation. It is difficult to find one that may show significant improvement over the optimal overrelaxation process if the inferences from the study of the solution of Laplace equation is any guide. Further substantial reduction of operation counts per iteration step is derived from cyclic processes built upon the Gauss-Seidel iterative procedure. If the field of computation constitutes p columns of q elements in each row with p $q \stackrel{\sim}{=} N$, the matrix B may be chosen block-lower-triangular so that each of the q blocks consists only the p (or q) elements in each column (row). Then B^{n-q+1} B^{n-q+2} ... B^n can be assigned as the lower triangular matrix in successive blocks with

zero elements everywhere else. This is the line Gauss-Seidel process operating on successive columns, (or rows). Such a line process can be accelerated by employing some proper acceleration parameter.

The line processes along columns and rows (diagonals or other convenient directions) may be employed in succession such as the sequence of operators $(B^{n-q-p+1}, \dots, B^{n-q})(B^{n-q+1}, \dots, B^n)$ and its cyclic repetition. A set of acceleration parameters may be employed with the cyclic column-row sequence. This is known as the alternating direction methods or the [6] method of Peaceman and Rachford who first demonstrated the power of such cyclic iterative methods for the solution of Laplace equations. Such line methods derive the benefit of less computational work from the basic fact that the operation counts of Gauss-Seidel process is proportional to the "square" of the vector length of the unknown. Thus the operational counts of a complete cycle is, with $p = q = N^{1/2}$ for example,

 $p \cdot q^2 + q \cdot p^2 = (p+q)pq \sim 2N^{3/2}$ (6.8)

compared with the N^2 for the point Gauss-Seidel process. This means a decrease of the operation counts per sweep by the factor $2/\sqrt{N}$, significant to the order of magnitude with $N=0(10^3)$. The extension of such cyclic process to problems in three space dimensions with $p \sim q \sim r \sim N^{1/3}$ is obvious. The total operational counts per cycle is $\sim 3N^{4/3}$ and the factor of operational counts reduction will be $3/N^{2/3}$. The preference of alternating direction iteration (ADI) or any such cyclic line iteration process over the point Gauss-Seidel relaxation process is clear. The success of reducing the overall computational effort in the solution of steady flow problems with such schemes requires, in addition, the appropriate choice of the

acceleration parameters suitable for the type of problems with the class of prescribed boundary data. This is where the uncertainty resides.

For the solution of Laplace equations, the optimal acceleration parameters and the maximum rates of convergence of these processes can be explicitly determined. The ADI process is certainly the most efficient.

The same is likely to be true for the integration of purely elliptical equations especially those with the Laplacian operator as the leading terms. For more complicated equations, including the equations of hydrodynamics, much depends on the ability of selecting the appropriate acceleration parameters for the problem at hand and on how the boundary conditions are implemented. For hyperbolic problems with discontinuous solutions as interior boundaries, success with the implicit methods is yet to be demonstrated.

4.4 Fractional Time and other Alternating Direction Methods

An alternating direction iterative method has been developed extensively in the Soviet Union by Yanenko, Marchuk, etc., known as the time splitting or fractional time step methods. The key idea is to split the operator as a sum of implicit difference operators, each of which will lead to an easily invertible tridiagonal matrix. The successive split operations in a complete cycle serves as a "weak" approximation of the original operator. They prefer unconditional computational stability and formal second order accuracy of the Crenk-Nicholson algorithm. This was illustrated in Equation (3.6) when θ takes the value $\frac{1}{2}$. Second order accuracy is needed since a first order accurate scheme can hardly meet the accuracy requirement of practical problems with the currently available computing machine. Its development and its relative merits pertinent to the gas dynamic

applications are presented below.

Consider first the equation

$$\frac{\partial \phi}{\partial r} + L\phi = 0 \tag{4.9}$$

where L is a linear spatial differential operator explicitly independent of time t. Discretized with the Crank-Nicholson algorithm which is second order accurate in both time and space,

$$\frac{\phi^{n+1} - \phi^n}{\Delta t} + L \left(\frac{\phi^{n+1} + \phi^n}{2} \right) = 0 \tag{4.10}$$

Let I be the identity operator, we have

$$(I + \frac{\Delta t}{2} L) \phi^{n+1} = (I - \frac{\Delta t}{2} L) \phi^n$$

or

$$\phi^{n+1} = (I + \frac{\Delta t}{2} L)^{-1} (I - \frac{\Delta t}{2} L) \phi^n = C \phi^n$$

For the simple heat diffusion equation $L_x \sim -\sigma \frac{\partial^2}{\partial x^2}$, the matrix $(I + \frac{\Delta t}{2} L_x)$ is tridiagonal and the spectral radius of the matrix C is obtained as

$$\rho(C) = \frac{1-S \psi}{1+S \psi}$$
 with $\psi = 4 \sin^2(\frac{\pi}{2} \frac{1}{j+1})$

when $0 \le x = j\Delta x \le (J+1)\Delta x$

Thus

$$||\phi^{n+1}|| \le \frac{1-S\psi}{1+S\psi} ||\phi^n|| \le \cdots \le (\frac{1-S\psi}{1+S\psi})^n ||\phi^o||$$

which establishes the boundedness and unconditional stability. Indeed with $\Delta t/\Delta x$ taken as constant, the computational error is bounded $||e|| \leq ||e_0|| + O(\Delta x^2)$. When the C.F.L. condition $\Delta t/\Delta x \leq 1$ for the wave equations is satisfied, this scheme was expected to work for both the diffusion and the wave equations, and was hoped to work for the Navier-Stokes

type equations at least for the 1-D case, (which is not necessarily true as is shown in section 3.2 for other difference algorithms).

Consider now the heat diffusion problem in three space dimensions

$$\frac{\partial \phi}{\partial t} - \sigma \left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \right) \phi = 0.$$

Now L = L_x + L_y + L_z or L₁ + L₂ + L₃. While the operations $(I + \frac{\Delta t}{2} L_x)^{-1}$ can be easily inverted, the combined matrix $[I + \frac{\Delta t}{2} (L_x + L_y + L_z)]$ is no longer tridiagonal, and although highly sparse, cannot be simply inverted. So the equation is to be integrated in three successive steps for the time interval $t_n \le t \le t_{n+1}$ and is formally designated as the fractional time steps $t_{n+1/3}$, $t_{n+2/3}$ and $t_{n+3/3} = t_{n+1}$. For each step at $t_{n+3/3}$ the Crank Nicholson algorithm,

$$\phi^{n+\alpha/3} = (1 + \frac{\Delta t}{6} L_{\alpha})^{-1} (1 \frac{\Delta t}{6} L_{\alpha}) \phi^{n+\frac{\alpha-1}{3}}$$

is used, thus:

$$\phi^{n+1} = \frac{3}{n!} (I + \frac{\Delta t}{6} L_{\alpha})^{-1} (I - \frac{\Delta t}{6} L_{\alpha}) \phi^{n}$$

$$= \{I - \Delta t L + \frac{\Delta t^{2}}{2} [L^{2} + \sum_{\alpha=1}^{3} \sum_{\beta=\alpha+1}^{3} (L_{\alpha}L_{\beta} - L_{\beta}L_{\alpha}) + \dots] + 0(\Delta t^{3})\}\phi^{n}$$
and is
$$= (I + \frac{\Delta t}{2} L)^{-1} (I - \frac{\Delta t}{2} L) + 0(\Delta t^{3})\}\phi^{n}$$
if L_{α} L_{β} is commutable.

Thus the split difference scheme will be second order accurate if the split operators are commutable. Otherwise, it is only first order accurate. When such commutativity of split operators for different dimensions (x,y & z) is not true, the split scheme of only first order accuracy can give second

order accurate results in two cycles if the cycle is repeated in the opposite direction. For the two consecutive cycles, i.e.

$$\phi^{n+1} = \prod_{\alpha=1}^{3} (I + \frac{\Delta t}{6} L_{\alpha})^{-1} (I - \frac{\Delta t}{6} L_{\alpha}) \phi^{n}$$

and

$$\phi^{n+2} = \prod_{\alpha=3}^{1} (1 + \frac{\Delta t}{6} L_{\alpha})^{-1} (1 - \frac{\Delta t}{6} L_{\alpha}) \phi^{n+1}$$

the two non-commutative terms would cancel and the second order accuracy is resumed for non-commutative operators L_{α} 's. This statement will be true even if L_{α} 's involve differential operators with varying coefficients or even depend on ϕ for gas dynamic quasi-linear equations so long as such coefficients are smooth and properly treated.

For unconditional stability, it is required that the operator L and all the split operators L_1, L_2 & L_3 are semi-positive definite, that is, the inner product of $(L\phi,\phi) \geq 0$ for any arbitrary function and defined over the entire field of computation. This condition is crucial in securing unconditional computational stability. Take the norm of ϕ^{n+1} and define the norms of an operator as the natural norm deduced from any vector norm then

$$||\phi^{n+1}||^2 = \frac{[(1+\frac{\Delta t}{2}L)^{-1}(1-\frac{\Delta t}{2}L)\phi^n, (1+\frac{\Delta t}{2}L)^{-1}(1-\frac{\Delta t}{2}L)\phi^n]}{(\phi^n,\phi^n)} \cdot ||\phi^2||^2$$

Defins

$$\left(1+\frac{\Delta t}{2}L\right)^{-1}\phi^n=\xi^n$$

then

$$||\phi^{n+1}||^2 = \frac{||(I - \frac{\Delta t}{2} L) \xi^n||^2}{||(I + \frac{\Delta t}{2} L) \xi^n||^2} ||\phi^n||^2 = \Lambda^2 ||\phi^n||^2.$$

Here

$$\begin{aligned} ||(\mathbf{I} - \frac{\Delta t}{2} \mathbf{L})\xi^{n}||^{2} &= [\mathbf{I} - \frac{\Delta t}{2} \mathbf{L})\xi^{n}, \ (\mathbf{I} - \frac{\Delta t}{2} \mathbf{L}) \xi^{n}] \\ &= ||\xi^{n}||^{2} - \Delta t \ [\mathbf{L}(\xi)^{n}, \xi^{n}] + \frac{\Delta t^{2}}{4} ||\mathbf{L}(\xi^{n})||^{2} \\ ||(\mathbf{I} + \frac{\Delta t}{2} \mathbf{L}) \xi^{n}||^{2} &= [(\mathbf{I} + \frac{\Delta t}{2} \mathbf{L})\xi^{n}, \ (\mathbf{I} + \frac{\Delta t}{2} \mathbf{L}) \xi^{n}] \\ &= ||\xi^{n}||^{2} + \Delta t [\mathbf{L}(\xi^{n}), \xi^{n}] + \frac{\Delta t^{2}}{4} \ ||\mathbf{L}(\xi^{n})||^{2}. \end{aligned}$$

This Λ^2 corresponds to the square of the spectral radius $\rho(C)$ for the simple 1-D heat diffusion problem with the Crank-Nicholson algorithm. Since both $||\xi||^2$ and $||L(\xi)||^2$ are positive and $\Delta t > 0$, the amplification factor Λ^2 will be \geq or < than unity depending on whether $(L(\xi), \xi) \geq$ or < 0

The successive application of the split operator at each step leads to

$$||\phi^{n+1}||^2 = \Lambda_1^2 \Lambda_2^2 \Lambda_3^2 ||\phi^n||^2$$

The conditions for Λ_1^2 , Λ_2^2 & Λ_3^2 to be less than or equal to unity are equivalent to the semi-positive definitions of the split operators L_1 , L_2 & L_3 , i.e. $(L_{\alpha}\phi,\phi) \geq 0$ for $\alpha=1,2,3$. It is true then that unconditional stability results if all operators L_{α} of L are semi-positive definite, i.e. $(L_{\alpha}\phi,\phi) \geq 0$. This semi-positive definiteness is a sufficient condition for stability for the entire cycle but not a necessary one.

Now if this restriction of semi-positive definiteness is to be assured this will practically limit its applicability to the simple diffusion equation or the Laplace equation in rectangular domain and for the Dirichelet problems. It is only a matter of intuition that the method should be applicable to a wider class of circumstances than those for which proofs could be given. The situation is really no better off than what was encountered for the explicit schemes on the question of stability. There

is indeed not even a necessary criterion of computational stability of this split method comparable to the von Heumann stability criterion for explicit schemes.

In the theoretical treatment of the gas dynamic problems, (Marchuk, Yamenko, etc.) the semi-positive definite condition is satisfied by imposing the special "periodic" boundary conditions to the problem; in which case it is clear that

$$(L\phi,\phi)=0$$

so that $\Lambda^2 = \Lambda_1^2 = \Lambda_2^2 = \Lambda_3^2 = 1$, i.e. the norm is preserved, i.e.

$$||\phi^{n+1}|| - ||\phi^{n}|| - ... - ||\phi^{0}||$$

This appears to be an excellent feature for initial value problems. But it also implies that whatever error in the initial data (if it is a guess) will not decrease in the mean square norm, for example. The splitting scheme should not be used to obtain steady state solutions with the periodic boundary condition because the results will never be better than the initial guess within the integral norm.

For treating practical problems the physical significance of this stability requirement of $(L\phi,\phi)\geq 0$ need be more carefully examined. Post-multiply with ϕ the equation

$$\frac{\partial \phi}{\partial t} + L \phi = 0$$

and sum (or integrate) over the entire field of computation to give

$$\frac{\partial}{\partial r} ||\phi|| + (L\phi, \phi) = 0$$

i.e.

$$\frac{\partial}{\partial t} ||\phi||^2 = - (L\phi, \phi)$$

If L is semi-positive definite, i.e. $(L\phi,\phi) \geq 0$, then $\frac{\partial}{\partial t} ||\phi||^2 \leq 0$. This of course implies the boundedness of the solution ϕ at all times and a decreasing sequence of || \phi ||^2. Now the gas dynamic equations in primary physical variables are such conservation laws for mass, momentum, and energy. Lo is the net fluxes of these conserved quantities out of unit physical volume. If \$\phi\$ and hence L\$\phi\$ are periodic over the parallelopided in the physical space to secure $(L\phi,\phi)=0$, then the outflux and the influx across the boundary of computation exactly balances. Thus with of identified as mass, momentum and energy, this condition excludes the loss of mass, momentum, and energy throughout the entire field of computation. This means that the computed results should not be expected to show body forces acting on some immersed body or heat transfer to and from the body. If there should be any in the computed results with periodic boundary conditions, whatever lift, drag and heat transfer as may be present in the computed results originate from some computational artifices and are physically meaningless.

If now the flow field is computed with periodic (asymmetric) boundary conditions in the transverse plane, then $\Lambda_2^2 = \Lambda_3^2 = 1$. A deficit of the out-flux L ϕ and a positive ϕ will render ($L_1\phi,\phi$) ≤ 0 and hence $\Lambda_1^2 > 1$ when there is a body drag (or energy sink to the body). Hence $\Lambda^2 = \Lambda_1^2 > 1$ and the computation will be "unstable". To secure computational stability under the circumstances, it is necessary to modify the boundary conditions in the transverse plane so that Λ_2^2 & Λ_3^2 are sufficiently smaller than unity to render Λ_1^2 Λ_2^2 Λ_3^2 < 1. Guidance is badly needed here for handling these boundary conditions properly to secure computational stability with

the split schemes. And even if computational stability is achieved by some means, there is little idea how the results of such important quantities as body drag, lift, and heat transfer, as calculated, will compare with the physical situation.

The fractional time step method outlined above was not meant to be applied to the steady state problems because each of the iterative solutions, $\phi^{n+1/3}$, $\phi^{n+2/3}$ and ϕ^{n+1} , satisfy different equations, none of them approximates the steady state equations. Even if the exact steady state solution of a given problem is substituted and used as the initial data, the fractional time step method will generate solutions for different fractional steps which will not quite settle down to some sort of a steady state limit. This situation can be remedied by retaining those terms, dropped in the fractional step method, to be evaluated with the previous or otherwise known iterate, for example,

$$\phi^{n + \alpha/3} = (I + \frac{\Delta t}{6} L_{\alpha})^{-1} \{I + \frac{\Delta t}{6} L_{\alpha} - \frac{\Delta t}{3} \sum_{\alpha} L_{\alpha}\} \phi^{n + \alpha-1}$$

which would indeed be the same as the alternating direction iterative solution of the implicit formulation of the steady state problem with $B = (I + \frac{\Delta t}{6} L_{\alpha}) \text{ and } A = \frac{\Delta t}{3} L = \frac{\Delta t}{3} \sum_{\alpha} L_{\alpha} \text{ given as equation (4.4a)}$ This method is then similar to the Douglas and Gumn's extension of Peaceman-Rachford's Alternating Direction methods for the solution of steady state problems. With the additional terms, it is not possible to conjecture what the stability behavior of the difference formalation and the convergence rate will be. Some experience of the research group at Langley Research Center, NASA (the author is grateful for this private communication) indicates that the overall computational effort of using such schemes for the numerical integration of the Navier-Stokes Equations

for some mixed supersonic-subsonic flow fields is much larger than that experienced by the author on similar problems with explicit formulation.

While no generalization is implied, the fundamental reasons expounded in this and the previous sections and some practical experience may serve an appropriate caution against being over optimistic to the advantage of such implicit methods.

The fractional step method was developed primarily for time dependent flow problems. The split operator L_{χ} , for example, can be split further as $L_{\chi} = L_{\chi c} + L_{\chi v}$ where $L_{\chi c}$ is the convective part and $L_{\chi v}$ the viscous part respectively of L_{χ} . In this manner, each comentum equation is split into 6 parts. Each of the 6 parts gives rise to either a wave operator or a diffusion operator. The question of rendering a stable computation for each step is such simplified although the split scheme is not unconditionally stable under realistic boundary conditions. There will be some inconsistencies in the formulation that can be remedied by including some higher order terms. The process rapidly becomes more complex especially when higher order temporal accuracy is desired. All the complexities must be weighed in the light of other difficulties in treating time dependent computations for 3-D flows. Such developments in dynamic meteorology and oceanography can be important in aerospace applications in the near future if not of much immediate concorn.

V. ACCURACY AND CONSERVATIVE FORMULATION

The physical conservation laws of mass, momentum and energy are established over arbitrary macroscopic volumes of a homogeneous fluid. By reducing the volume to a macroscopically small "point", but a microscopically large domain to justify the continuum model, the Navier-Stokes partial differential equations were derived as a convenient mathematical relation governing smooth point functions in the flow field. Now, in the interest of determining some flow fields, the Navier-Stokes equations are discretized into a system of difference equations for finite elements of spatial domains to facilitate the numerical integration of the partial differential equations system. Such difference equations may as well be obtained directly from the consideration of the fundamental physical laws for such finite, discrete, spatial domains with the help of interpolation formulas. It is, however, more common that discretization is effected by replacing a differential coefficient with difference quotients according to some truncated Taylor series to some order of accuracy. The errors associated with the interpolation formula or the truncated Taylor series are called truncation errors, some of which are given as e, in Tables I and II. The mathematical requirement of consistency means only that the truncation error will vanish as Δt , $\Delta x + 0$.

The conservation laws for each finite spatial element are properly approximated to some formal order of accuracy, according to the truncation error, by the difference equations deduced in either manner mentioned above. When the difference forms of such conservation laws are summed

and examined over a large but arbitrary collection of such finite spatial elements, however, the conservation laws may be seriously violated. This is because the higher order small errors will accumulate to much large errors when summed over a very large number of the small discrete elements which add up to the finite domain of computation. Now for an appropriate description of a physical problem to the accuracy, say $O(\Delta x^2)$, it is primarily and essentially over arbitrary finite volumes, not only over the differential elements, that such conservation laws should be accurate to $O(\Delta x^2)$. If the truncation errors of the conservation laws in finite space is to be of $O(\Delta x^2)$, it must not accumulate when neighboring mesh cells are summed up. If the truncation errors are allowed to accumulate, the difference formulation should be higher order accurate so that the accumulation of such higher order small truncation errors over arbitrary mesh combinations throughout the field of computation will not exceed $O(\Delta x^2)$, for example. The difference form of Navier-Stokes equations, accurate uniformly to better than $O(\Delta x^2)$, is extremely cumbersome to construct and execute. With limited spatial resolution currently available, it is imperative to prevent or limit the accumulation of truncation errors.

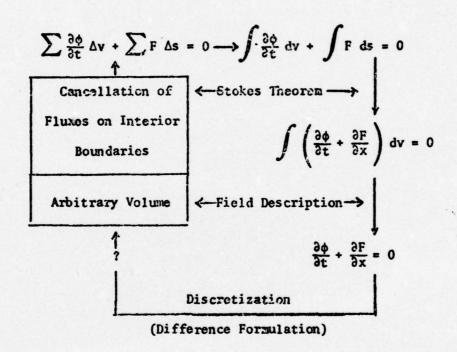
It is highly commendable to verify a posteriori, to what extent the computed results conserve the mass, momentum and energy over the entire field of computation. But this is not an alternative to the requirement of no accumulation of the truncation errors. The truncation errors are generally in the form of dipoles or quadruples rather than simple sources or sinks. They distort the local flow field much more than they cause apparent deviations in the overall mass, momentum and energy balances. The consequence of such dipoles and the like is indeed familiar to aerodynamicists. A circular cylinder in a uniform incompressible flow is

represented by a doublet. A thin airfoil or a thin wing in a subsonic or a supersonic flow is represented by some distribution of sources and sinks or dipole pairs within the framework of some linearized theory, known as the method of singularities. If a series of tiny little vanes or thin sheets are not to be tolerated in the test section of a windtunnel, such distributed dipoles arising from the truncation errors of every computational cell must be suppressed if not completely eliminated. Such suppression can be achieved with some attention paid to the formulation of the difference problem.

5.1 Conservative Difference Formulation

The conservation relations are written in divergence form as Equations (1.1) to (1.3) for the density ρ , the momentum ρu_i , and energy density per unit volume. They are the scalar components of the vector function V in Equation (1.6), etc. These five quantities will be considered as the "Primary Dependent Variables" in terms of which the physical laws are stated and the practical results desired. They provide the integrals of motion when proper initial and boundary data are provided over a specific but arbitrary volume. When neighboring volumes are summed, the contributions on their common boundary cancel identically so that the integrated conservation laws retain their identical form. This is the crucial property that enables the integral theorems of Stokes and Green to cast the conservation principles into field descriptions in terms of different variables (Fig. 2). An adequate approximation of the conservation laws in difference form should preferably retain this property at least to the order of accuracy required. Such a summable property is implicit in the mathematical abstraction of continuity and differentiability of the

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functions in question. Thus, the differential formulations in terms of different dependent and independent variables are all equivalent although the forms of the partial differential equations may be much different. This is not the case for the difference approximations of the conservation laws that may be formally "derived" from the varieties of forms of equivalent partial differential equations. This is because the difference functions over the mesh points or cells are discrete or at least not differentiable beyond a certain order. The summable difference formulation, in the sense that when cells in the field of computation are summed. the fluxes in the physical space (x;) of the primary dependent variables cancel identically along their common boundary will be called "Conservative Difference Formulation". The computational space need not be the physical space. The dependent variables computed need not be the primary ones. While the computation can be done in this manner, it is still the fluxes in the physical space and of the primary variables that are required to be summable for the conservative difference formulation.

For illustrative purposes, consider the discretization of the continuity relation from the integrated conservation law expressed in the primary variables ρ , ρ_u , and ρ_v in the two dimensional physical space (x,y) divided into uniform rectangular cells $\Delta x \Delta y$. $\rho_{j,k}$ is the average density of the fluid in the cell $j\Delta x$, $k\Delta y$. The net increase of mass in the cell during Δt is $(\rho_{j,k}^{n+1} - \rho_{j,k}^n)\Delta x \cdot \Delta y$. The mass fluxes of ρ_u and ρ_v should be evaluated on the boundary while ρ_u and ρ_v are known only as the average momentum of the fluid in the cells. Thus the boundary fluxes are evaluated through linear interpolation (but of second order accuracy) as the arithematic average of the mean momentum in neighboring cells. If increasing j and k are positive directions, the conservation of mass is stated as:

$$\left\{ (\rho_{j,k}^{n+1} - \rho_{j,k}^{n}) \Delta x \Delta y + \frac{\Delta t \Delta y}{2} \right\} \left[(\rho U)_{j+1,k}^{n} + (\rho U)_{j,k}^{n} \right] - \left[(\rho U)_{j,k}^{n} + (\rho U)_{j-1,k}^{n} \right]$$

$$+ \frac{\Delta t \Delta x}{2} \left\{ \left[(\rho V)_{j,k+1}^{n} + (\rho V)_{j,k}^{n} \right] - \left[(\rho V)_{j,k}^{n} + (\rho V)_{j,k-1}^{n} \right] \right\} = 0$$

$$(5.1)$$

For the neighboring cell (j-1)Δx·kΔy, the difference form of mass continuity relation can be obtained from (5.1) by replacing j by j-1. The two cells have a common boundary at $(j-\frac{1}{2})\Delta x \cdot k\Delta y$. The cut flux from the cell j-1,k crossing this common boundary is $\frac{1}{2}\{(\rho U)_{j,k}^n + (\rho U)_{j-1,k}^n\}$, which is identically the same as the in flux to the cell (j,k). When the two mass continuity equations (5.1) for the cells (j,k) and (j-1,k) are added, the flux terms across the common boundary cancel out. The resulting difference equation is identical with the one that will be obtained when the conservation law is applied directly to the combined cells and is accurate to $O(\Delta x^2)$. The addition of other neighboring cells behave in the same manner. Similar results will be obtained for the momentum and the energy relations. Thus a conservative difference formulation accurate to $O(\Delta x^2)$ is obtained. It is easily verified that the same difference formulation will be obtained with the forward time, centered spatial difference algorithm applied to the differential equations system (1.1) to (1.3) written in divergence form. Indeed the first order accurate algorithm of backward or forward spatial difference will also yield a conservation difference formulation, but of first order accuracy, i.e., O(Δx) provided that the differential equation is discretized in divergence form and that the physical space is divided into uniform spacing.

If the continuity equation should be written in expanded form for discretization such as: $u \frac{\partial \rho}{\partial x} + \rho \frac{\partial u}{\partial x}$ for the net mass flux in the x-direction, the centered space difference algorithm can represent the net x-flux as

$$\frac{\Delta t \Delta y}{2} \left[U_{j} (\rho_{j+1} - \rho_{j-1}) + \rho_{j} (U_{j+1} - U_{j-1}) \right]$$
 (5.2a)

or
$$\frac{\Delta t \Delta y}{4} \left[(U_{j+1} + U_{j-1})(\rho_{j+1} - \rho_{j-1}) + (\rho_{j+1} + \rho_{j-1})(U_{j+1} - U_{j-1}) \right]$$

The in flux to the cell (j,k) from the cell (j-1,k) crossing the boundary at $(j-\frac{1}{2})\Delta x$ is respectively:

$$\frac{\Delta t \Delta y}{2} \left[U_{j} \rho_{j-1} + \rho_{j} U_{j-1} \right]$$
 (5.3a)

or
$$\frac{\Delta t \Delta y}{4} \left[(U_{j+1} + U_{j-1}) \rho_{j-1} + (\rho_{j+1} + \rho_{j-1}) U_{j-1} \right]$$
 (5.3b)

The out flux from the cell (j-1,k) into the cell (j,k) crossing the same common boundary as may be obtained from Equation (5.2a)(5.2b) by putting j + j-1 is respectively

$$\frac{\Delta t \Delta y}{2} \left[U_{j-1} \rho_j + \rho_{j-1} U_j \right]$$
 (5.4a)

or
$$\frac{\Delta t \Delta y}{4} \left[(U_j + U_{j-2}) \rho_j + (\rho_j + \rho_{j-2}) U_j \right]$$
 (5.4b)

The out flux (5.4a) is identical as the in flux (5.3a) and will cancel each other when the two cells are summed. Thus the difference algorithm (5.2a) will lead to a conservative difference formulation with the differential equation not written in divergence form. The out flux (5.4b) is different from the in flux (5.3b). When the two cells are summed up, they do not cancel completely but produce a net mass source along the common boundary, but in the interior of the pair of cells, with the magnitude proportional to Δx . This is formally negligible in a second order accurate

algorithm but renders the difference formulation from the algorithm (5.2b) not summable and not conservative. Even if such errors are accumulated randomly over the field of computation with $1/\Delta x^2$ meshes, the accumulated truncation error will be of $O(\Delta x)$ rather than $O(\Delta x^2)$. If the first order accurate forward or backward spatial difference algorithm is used, the net x-flux will be

$$\frac{\Delta t \cdot \Delta y}{2} \left[U_j (\rho_j - \rho_{j-1}) + \rho_j (U_j - U_{j-1}) \right]$$
 (5.5a)

or
$$\frac{\Delta t \cdot \Delta y}{2} \left[U_j (\rho_{j+1} - \rho_j) + \rho_j (U_{j+1} - U_j) \right]$$
 (5.5b)

Neither of the two will lead to conservative difference formulation even at the accuracy of $O(\Delta x)$. The above examples demonstrate that both the center difference algorithm and the divergence form of the differential equation are conducive to the conservative difference formulation with uniform mesh size in physical space. The difference formulation based on integrated conservation laws even with linear interpolation on the other hand, leads straightforwardedly to conservative difference form of second order accuracy.

Consider now the effect of newwaiform mash sizes in physical space with

$$\frac{(\Delta x)_{j+1}}{(\Delta x)_{j}} = \eta_{j+\frac{1}{2}} \quad \text{and} \quad \frac{(\Delta x)_{j}}{(\Delta x)_{j-1}} = \eta_{j-\frac{1}{2}}$$

using the integrated conservation laws and linear interpolation. The net flux into the cell at $j\Delta x$ during the time interval Δt is obtained in a straightforward manner, illustrated here only for x-fluxes:

$$+ \Delta t \cdot \Delta y \left[\frac{\eta_{j+\frac{1}{2}}}{1 + \eta_{j+\frac{1}{2}}} \left(\rho U \right)_j + \frac{1}{1 + \eta_{j+\frac{1}{2}}} \left(\rho U \right)_{j+1} \right]$$

$$- \Delta t \Delta y \left[\frac{\eta_{j-\frac{1}{2}}}{1 + \eta_{j-\frac{1}{2}}} (\rho U)_{j-1} + \frac{1}{1 + \eta_{j-\frac{1}{2}}} (\rho U)_{j} \right]$$
 (5.6)

The first bracket represents the out flux from cell j. The second bracket represents the in flux to cell j. If, in the first bracket, j is replaced by j-1, then the out flux from the cell at $(\Delta x)_{j-1}$ becomes identical as the in flux into the cell at $(\Delta x)_j$ across their common boundary. They cancel each other when the two cells are summed. Thus the algorithm (5.6) in physical space will lead to a conservative difference formulation despite the variable spacing in physical space. The algorithm (5.6) clearly indicates how the centered spatial difference algorithm should be modified to accommodate the variable physical spacing in order to achieve the conservative difference formulation and the second order accuracy. This particular combination of the weighted average of $(\rho U)_{j+1}$, $(\rho U)_j$, and $(\rho U)_{j-1}$ is, however, not obvious from the point of view of discretizing $\frac{\partial}{\partial x}$ (ρu) with the second order accuracy through Taylor series expansions.

It is common that variable mesh sizes in physical space are accomplished through some transformation of the independent variables, $x = x(\xi)$ or inversely $\xi = \xi(x)$. The difference formulation is then derived from the transformed differential equation by discretization over uniform mesh spacing $\Delta \xi$ in the transformed ξ -space according to some difference algorithm. This transformation of the spatial coordinates is often suggested by the desire of bringing the boundaries into coordinate lines such as $\xi \sim x/1+x$ so that $x = \infty$ corresponds to $\xi = 1$ or the use of spherical, cylindrical or other convenient body coordinates dictated by the contour of the solid

body present in the flow field. The disretization in the transformed ξ -space in an intuitive manner is not likely to produce a conservative difference formulation. Even with uniform mesh spacing $\Delta \xi$, the cancellation of in flux and out flux is not assured in the physical space although it is achieved in the transformed space. This is because of the presence of the metric coefficients.

Consider the mass continuity relation in the cylindrical polar coordinates (r, θ, z) :

$$\frac{\partial \rho}{\partial t} + \frac{1}{r} \frac{\partial}{\partial r} (r\rho u) + \frac{1}{r} \frac{\partial}{\partial \theta} (\rho v) + \frac{\partial}{\partial z} (\rho w) = 0$$
 (5.7)

where u, v, and w are the radial, azimuthal and axial velocity components. Even if the mesh spacings Δr , $\Delta \theta$, and Δz are uniform and the central space difference algorithm is adopted. There is left the question how the metric coefficient r should be treated in discretizing Equation (5.7) to obtain a conservative difference form. Now the integrated conservation relations in the physical space with curvilinear coordinates stands as

$$\Delta \mathbf{r} \cdot \Delta \mathbf{z} \cdot (\mathbf{r}_{j} \Delta \theta) \cdot \Delta_{\mathbf{t}}(\rho)$$

$$= \Delta \mathbf{t} \cdot \Delta \mathbf{z} \ \Delta_{\mathbf{r}}(\rho \mathbf{u} \mathbf{r} \cdot \Delta \theta) + \Delta \mathbf{t} \cdot \Delta \mathbf{z} \cdot \Delta \mathbf{r} \Delta_{\theta}(\rho \mathbf{v})$$

$$+ \Delta \mathbf{t} \cdot \Delta \mathbf{r} \cdot (\mathbf{r}_{j} \Delta \theta) \cdot \Delta_{\mathbf{z}}(\rho \mathbf{w}) \tag{5.8}$$

where Δ with subscript r, θ , or z stands for the net flux of the quantity in the parenthesis in some difference form. The left hand side of Equation (5.8) stands for the net increase of mass in the volume element. If the flux terms on the right hand side are expressed either in the form (5.1) for uniform mesh sizes or in the form (5.6) for nonuniform mesh sizes, for

example, the difference form of the continuity equation will be conservative or summable. Thus the metric coefficient r arising from the volume element should be treated as r, while the metric coefficient r arising from the surface element should be treated differently for the in flux and the out flux surfaces depending upon the specific difference algorithm. It appears therefore that the conservative difference formulation can be more conveniently obtained by considering the integrated conservation relations in the physical space despite the curvilinear coordinate system that may have to be adopted.

The treatment of the conservation relations of the vector momentum is considerably more complicated than that of the scalar mass because of the stress terms and the inertia terms due to curvature and because of the need of considering the appropriate vector components. Complicated as it may be, the flux terms can be clearly identified and conservative difference formulations can be obtained. Often it is desirable for achieving a simpler difference formulation by relaxing the condition of identical cancellation of the in flux and out flux crossing the same common cell boundary. The more lenient requirement may be that the in flux and out flux crossing the same boundary differ by a sufficiently higher order small quantity to provide for some accumulation and possibly supplemented by their vanishing over a group of say four neighboring cells. This may be permissible since the ultimate objective of the conservative difference formulation is to prevent undue accumulation of truncation errors over finite volumes to cause serious deterioration of the accuracy of the computation.

With conservative difference formulation, the accumulated truncation error E_T of a set of calculations can be estimated to the order of magnitude at any point within the field of computation. Moreover, the error of the computed results at a point can be separated into two parts:

(i) the truncation error E_T and (ii) the boundary error at the point caused by the errors on the boundary of the field of computation although the difference problem is essentially non-linear.

5.2 Houristic Error Estimate and Accuracy

For a computed result to be practically useful it is essential to have some idea of its accuracy. The study of the accuracy question has. however, been little explored. This may be due partly to the preoccupation with stability questions and partly to the difficulty of constructing an upper bound of the error of a computation for the type of initial boundary value problems of fluid dynamics. It may be possible that those convergence proofs which naturally include the estimate of the error bounds will be extended from the periodic boundary value problems to more realistic boundary conditions as applied to the Navier Stokes equations. In practice such a difficult and complicated a-priori rigorous error estimate is not necessary. Heuristic, a-posteriori rough error estimates will often suffice. Indeed, it would be preferable to have the estimate simple and generally applicable although not rigorous and not so precise. The nonlinear Burgers' equation is therefore conveniently adopted for analysis as a one-dimensional model of the Navier-Stokes equations. As was shown in Section (3.2), it is a useful model for stability analysis, being quasi-linear and with both wave and diffusion characteristics. It is also convenient for the study of accuracy because many exact solutions

are known, with which the computational errors can be quantitatively evaluated and compared with theoretical estimates.

The Burgers' equation, in dimensionless form is

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{1}{Re} \frac{\partial^2 u}{\partial x^2}$$
 (5.9)

with a steady state solution

and

$$u(x) = -\alpha \tanh (\alpha R_e x/2)$$
 (5.10)
having $u(x=0) = 0$ $u(x=-1/2) = 1$
and $|u(x=\pm \infty)| = \alpha = 1/\tanh (\alpha R_e/4)$

This steady state solution in the range of $-1/2 \le x \le 0$ has been calculated as the long time limit of the temporal problem via several difference algorithms. The quasi-linear term $u \frac{\partial u}{\partial x}$ is always treated in the divergence form $\frac{\partial}{\partial x}$ (u²/2) with

$$\left(\frac{U^{2}}{2}\right)_{j+\frac{1}{2}} = \left[\left(U_{j+1}^{2} + U_{j}^{2}\right) + aU_{j+1} U_{j}\right]/_{2(2+a)}$$

$$\Delta\left(\frac{U^{2}}{2}\right)_{j} = \frac{1}{\Delta x} \left[\left(\frac{U^{2}}{2}\right)_{j+\frac{1}{2}} - \left(\frac{U^{2}}{2}\right)_{j-\frac{1}{2}}\right]$$
(5.11)

Here "a" is a parameter. The simple centered spatial difference corresponds to a = 0. The center spatial difference in non-divergence form results when a = 0, in which case,

$$\Delta \left(\frac{U^2}{2}\right)_{j} = \frac{U_{j}(U_{j+1} - U_{j-1})}{2\Delta x}$$
 (5.12)

If it is presumed that an approximate steady state solution $U(t,x,\Delta t,\Delta x)$ will be reached, which departs only slightly from the genuine solution(5.10), a linearized differential equation for the error can be derived and solved. The linearization permits the separation of the errors as originated from various sources, i.e., as the sum of the truncation errors E_T and the boundary errors E_b . The difference equations derived from (5.11) are all nonlinear but conservative and permit the separation of the truncation and the boundary errors with the cumulative truncation errors E_T remain of the order of the local truncation error.

The linearized analysis shows that E_T at any point in the field of computation is proportional to $(Re_{\Delta X})^2$ for the second order accurate conservative difference formulations derived from (5.11). Here $Re_{\Delta X}$ is the Reynolds number based on the length Δx and the velocity difference between the point x=0 with maximum velocity gradient and the point x=1 nearly the asymptotic velocity. For a quantitative estimate of the E_T ,

$$\frac{E_{T}}{(Re_{A})^{2}} = M_{0}E_{0} + \frac{M_{1}E_{1} + (1+3a)M_{2}E_{2}}{2+a} + \frac{M_{3}}{2}E_{3}$$
 (5.13)

where Mo is the constant defining the steady state criterion

$$\sup_{j} \left[U_{j}^{n+1} - U_{j}^{n} \right] < M_{o} \Delta x^{3}$$

 $M_1(Re_{\Delta x})^2$ and $M_2(Re_{\Delta x})^2$ are the coefficients of the truncated quasi-linear convective terms and $M_3(Re_{\Delta x})^2$ is that of the truncated viscous terms. M_1 , M_2 , and M_3 are expected to be of O(1) for reasonable difference algorithms and for reasonably smooth solutions. E_0 , E_1 , and E_3 are universal functions of the genuine solution u(x) that vanish on both

boundaries and have their absolute magnitudes less than 0.1. Thus the truncation errors E_T are expected to be of the order of $(Re_{\Delta x})^2/10$ for the second order accurate schemes. Actual computations with $M_0 = O(\Delta x)^4$ and $\Delta x = 1/20$ for various schemes verified the quantitative values of Equation (5.13) and the dependence of E_T on $(Re_{\Delta x})^2$.

For $Re_{\Delta x} = O(1)$ and all the finite values of a = O(1) tested, the following estimate of the maximum absolute truncation errors is valid

$$E_T < 3 \times 10^{-2} (Re_{\Delta x})^2$$
 (5.14)

This simple formula is therefore recommended as a preliminary estimate of the bounds of the truncation errors of second order accurate conservative difference formulation. With non-conservative difference formulation, the truncation errors can accumulate and become considerably larger than the estimate given by Equation (5.14).

The boundary errors in the field due to a fractional error ε_b of the boundary value is given by the linearized analysis as:

$$\mathbf{E}_{\mathbf{R}} = \boldsymbol{\varepsilon}_{\mathbf{h}} \mathbf{E}_{\mathbf{h}} \tag{5.15}$$

where E_h is a universal function that is unity on the boundary where the erroneous boundary condition is applied, and decays very slowly toward the other boundary where it vanishes. The decay is so slow that the error retains more than half its value until within the last tenths of the field of computation near the other boundary (note that E_h is plotted against u(x) in Fig. 2 of Ref. 10) depending upon the magnitude of the Reynolds number.

For Neumann boundary conditions, the boundary error is still given by Equation (5.15) but ϵ_h is evaluated as

where ε_b^{\dagger} is the fractional error of the spatial derivative on the boundary. Within the framework of linearized estimate of errors, the superposition of (5.15) and (5.16) with proper coefficients will enable an estimate of the errors caused by a Cauchy-type condition. The boundary error at a given point in the field of computation will be the sum of the decayed boundary errors from both boundaries.

In multidimensional flow problems, it is presumed that the results of the previous model analysis may apply primarily in the direction along streamlines or nearly so. This leaves the estimate of the contributions of the boundary errors, from those portions of the boundary of the field of computation that are primarily parallel to the local streamline directions, yet to be accommodated. No helpful suggestions can be made here except to render a description as nearly correct as the physical situation suggests. In fact, the treatment of this portion of the computational boundary is one of the two outstanding difficulties that the author and his co-workers have experienced in various problems. (The other outstanding difficulty is the treatment of internal shockwaves to be explored in the next section.)

The decay characteristics described by the universal function E_h may be used where the one-dimensional model is appropriate. The various universal functions E_o , E_1 , etc. and E_h in the model results may be recognized as the "influence functions" describing the error propagation in the field of computation. They can be empirically established, a posteriori, by introducing a known error at a specific point (on the boundary for the specific boundary error and at chosen interior points

for truncation errors) and then computing the solution under the modulated condition. The difference of the two sets of solutions then gives the influence function E in question. Usually, during the development stage of a difference formulation for a given physical flow problem, such informations can be derived from preliminary results and can be used for the purpose of a-posteriori error estimate. Of course, a-posteriori determination of such influence functions are desirable to provide additional checks on the behavior of the computational program.

Without referring to any specific computational problem, the following general observations can be inferred from the model study. They are applicable only for the conservative difference formulation in which the truncation errors do not accumulate so that the truncation and the boundary errors can be treated separately and estimated by Equations (5.14) to (5.16).

- (1) The steady state criterion $|U_j^{n+1} U_j^n| < O(\Delta x)^n$ is sufficiently accurate in a second order accurate scheme.
- (2) The truncation error E_T is expected to be $\sim (Re_{\Delta X})^n$ for conservative difference formulation of nth order formal accuracy and the influence functions $E_{1,2}$, etc. are not likely to possess maximum magnitudes much less than 10^{-1} . With $Re_{\Delta X} > 1$ in the practical cases, maximum truncation error is not likely reduced appreciably from that of second order accurate scheme as may be estimated from (5.14).
- (3) Boundary errors cannot be efficiently reduced by reducing the mesh sizes. They decay vary slowly and are generally considerably larger than the truncation errors in practical cases with $Re_{\Delta x} = O(1)$. The primary effort required in achieving a reasonably accurate solution of the complicated practical problems lies in the sophistication in the treatment of the various boundary conditions. The field of computation and the choice

of coordinates should be properly defined to facilitate a more accurate implementation of the boundary conditions.

The general observations made above carry an important message to those interested in obtaining solutions for the complicated fluid dynamics problems with reasonable accuracy to suit practical purposes. Much attention should be paid to the formulation of the problem. Attempts to improve the accuracy of a numerical solution based on a poor formulation by extending the computation to satisfy more restrictive steady state criterion, with more refined mesh and even with the help of much larger and faster computers can prove to be not only expensive but frustrating.

A similar attempt was made for the time dependent flow. It was found that for flows with slow and memotonic temporal variations, the behavior of error propagation in the second order accurate conservative difference formulation is essentially similar to that described above for steady state problems. For oscillatory flows, conservation in the spatial space apparently fails to help. Test calculations for some simple damped oscillation as an exact solution of the Burgers' equation indicate the serious effect of the phase errors of different oscillatory components caused by the dispersive truncated terms. It has been suggested and illustrated that fourth order accurate difference algorithms will substantially improve the accuracy of the computed results beyond quite a few cycles of oscillations. It is, however, a tremendous task to compute with fourth order formal accuracy and uniformly for as complicated an equation system as the Navier-Stokes. [8,9,11]

5.3 Shock Wave and Artificial Viscosity

In all the previous discussions, the question of "non-smooth" or even "discontinuous" solutions is deferred. In problems of practical interest, shock waves and contact discontinuities are often the prominent features of the flow problems. The presence of such discontinuities, or generally regions of very large gradient, causes difficulties in their computation.

Discontinuous initial and boundary data are often imposed on purely elliptic or parabolic problems. They may cause oscillations in the vicinity of the boundary, but never very serious. This is because of the inherent nature of the system to smooth out any discontinuities in time and in space. The accuracy of the computed results may suffer somewhat according to the modulus of continuity of the functions involved, but can often be remedied by using a higher order accurate difference algorithm. This inherent tendency to smooth out any discontinuity can also be trouble-some, for example, in treating flow problems involving an interfacial discontinuity formed by two different fluid mediums, especially when the interface is not stationary; since initially sharp discontinuity diffuses in the course of the computation if not artificially maintained.

For hyperbolic problems, a discontinuity in the initial boundary data propagates into the field of computation and causes excessive computational disturbances downstream, particularly in its zone of influence. It also produces upstream influences. For the quasi-linear gas dynamic problems, a shock discontinuity can physically arise from a perfectly smooth boundary due to the coalesence of the smooth compression waves. Thus, when this flow field is computed with an algorithm that worked well

for smooth fields, quite severe oscillations can develop at approximately where the shock discontinuity would appear. Such escillations are fairly large, although not necessarily leading to the catastrophic divergence of linear instability. It may be that the amplitude of such shock induced oscillations are limited by the non-linear effects and the phenomenon may well be called nonlinear-instability, but certainly not in the sense of violating the requirement of boundedness discussed in Chapters II and III. Even if bounded, such oscillations are highly damaging to the accuracy of the results not only in the vicinity of the shock but over most of the flow field computed. Practical interest, on the other hand, is often centered in the vicinity of such shock discontinuity.

It is natural to treat the shock front or the interfacial contact discontinuity as an internal boundary and to compute the smooth solutions on both sides of the discontinuity separately. The jump conditions across the discontinuity will connect the two solutions together. This shock matching or shock fitting procedure is easily carried out in one space dimension for a known discontinuity, i.e., the magnitudes of the jumps and the speed of propagation of the discontinuous front into a homogeneous medium at rest or in uniform motion. If the shock should be propagating into a non-uniform medium or a homogeneous medium in non-uniform motion, the shock strength and speed will vary and the Hugoniot relations across the shock will have to be supplemented by some additional matching condition to be derived from the difference results in the vicinity of the shock front. It is often that oscillations appear on one or both sides of the shock discontinuity, likely as a result of the inaccuracies in the location of the shock and in the values of the functions in the

vicinity. The oscillations may be alleviated if the shock location is fixed at a mesh point and the mesh divisions are rezoned at every time or iterative steps. The computational procedure in terms of such shock coordinate rapidly becomes complicated.

In two space dimensions and with a curved shock of unknown shape and location, the computational details of such a shock matching procedure rapidly becomes more tedious and inaccurate. With fixed mesh points, the shock front is generally off the mesh points and it becomes difficult and highly inaccurate to determine the direction normal to the front in the matching process. The use of curvilinear shock coordinate is convenient and may possess other features for treating inviscid steady state flow problems with uniform supersonic flow on the upstream side of the shock front. 12 it is not suitable, however, for a shock wave imbedded in a nonuniform inviscid flow field. It cannot be implemented for viscous and inviscid flow fields involving more complicated shock configurations, such as shock intersections and Mach reflections or transonic shocks that terminate in the flow field. The tedious shock matching can be implemented in principle even for such complicated configurations although the procedure is too complicated to be manageable and the results so obtained are uniformly poor.

To avoid shock matching, v.Neumann and Richtmeyer introduced the artificial viscosity method for computing the shock propagation in an inviscid flow field. A quadratic viscous pressure term $\rho\alpha^2\Delta x^2 \left|\frac{\partial u}{\partial x}\right| \frac{\partial u}{\partial x}$, where α is a numerical constant chosen at convenience, is added to the differential equation before discretization. The quadratic dependence on the velocity gradient assures a rapid decay of the artificial viscous

the typical results of the calculation for one-dimensional shock propagation into a uniform field gives a sharp shock front, spreading over ~ 2 meshes and the calculated shock speed is within 0.1% of the correct value. But sizable oscillations develop in the downstream and over an extended range without appreciable damping (spatially and temporally). By increasing α to $\gtrsim 2$, the magnitudes of the oscillations are reduced but the shock front spreads wider, over 4 or more meshes. A reasonably smooth downstream solution is obtained only when α is so large as to be $O(\Delta x^{-1})$ and the shock front spreads over many meshes. By then the artificial viscous term is no longer small in the inviscid region and the apparently smooth results of computation fail to be a satisfactory approximate solution for the shock front.

The artificial viscosity method is physically sound, simply implemented and easily extended to multispace dimensions, formally by including dorivatives in other spatial dimensions. The large spread of the shock front and the induced oscillations generally become more objectionable, however. Many artifices can and have been devised to improve the appearance of the computed results. The artificial viscous term may be dropped when the gradient of velocity becomes less than a pre-assigned value, or the downstream oscillations may be suppressed or eliminated by some smoothing process or may be limited to a permissible magnitude about the mean through some filtering process. Excellent results can generally be obtained for simple test problems with known shocks. The merit of such procedures in computing shock propagation into non-uniform flow fields is yet to be demonstrated, particularly with respect to the accuracy of the smooth results.

[14]

The Lax-Wendroff treatment of shock wave utilizes the fact that the hugoniot relations are simply the conservation laws integrated over the discontinuity. Thus, with the inviscid equations written in divergence form for the physically conserved quantities, shock matching can be avoided since the difference equations for such conserved quantities are indeed the approximate form of the hugoniot relations. (Note that the divergence form of the transformed dependent variables does not help.) One dimensional computations show that it leads to a quite sharp shock front (~20x) and accurate shock speed. But sizable oscillations are generated at the shock front although rapidly damped to disappear within 8 to 10 meshes from the front. The dissipation is derived from the dissipative term $\Delta x^3 \cdot r(1-r^2) \frac{\partial^4 u}{\partial x^4}$ with $r = u\Delta t/\Delta x$ which may be visualized as the artificial viscosity that spreads out the shock front. The quadratic viscous terms adopted by v. Meumann and Richtmeyer does not appear to provide as much damping of the shock induced oscillations as this linear viscous term. The peak amplitude of this shock induced escillation near the front is often larger although more rapidly damped than those from the quadratic artificial viscous term. Additional artificial viscous terms are often introduced to reduce the amplitude of such oscillations.

The introduction of artificial viscous terms into the differential equation before discretization is fundamentally not much different from dropping those higher order terms in the truncated Taylor series in the discretization process. Such viscous terms contribute to the stability of the difference formulation. Thus artificial viscosity is very widely employed for problems without shocks. Such artificially introduced viscous terms are often substantially larger than the Navier-Stokes

viscous stress terms evaluated with the physical viscosity coefficient of the fluid. This is justifiable for the solution of inviscid flow problems, i.e., the flow problems visualized as the asymptotic limit of negligible viscous stress terms, so long as the contributions of the artificial viscous terms are "negligibly small" compared with the contributions from the inviscid terms and the somewhat spread out shock front is visualized as a "sharp" discontinuity. Such a situation is clearly not tolerable for viscous flow problems because the effect of the fluid viscosity will be overshadowed by the effect of the pseudo viscosity.

There are many numerical solutions of the Navier-Stokes equations, some with first order accurate algorithms, some with second order accurate algorithms but with large artificial viscous terms, at large Reynolds numbers based upon fluid viscosity of the order of 10⁶. These computed [15] results are very insensitive to the large fluid Reynolds numbers. This is understandable since the pseudo-viscosity in such calculations are substantially larger than the real fluid viscosity, and changes in the fluid Reynolds number will not significantly alter the effective Reynolds number of the computational results based on the total viscosity included in the difference formulation. If one wishes to evaluate quantitatively the viscous effects, both the artificial viscous term introduced into the differential equations system and the pseudo viscous terms implicit in the difference form should remain substantially less than the fluid viscous term. Thus for viscous flow problems, artificial viscosity terms of the type used by v.Neumann and Richtmeyer should satisfy

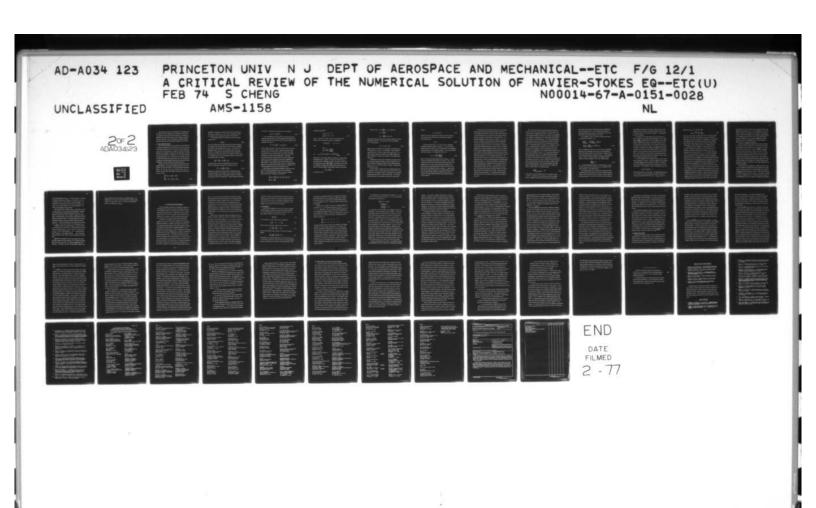
$$\alpha^2 \Delta x^2 \left(\frac{\partial u}{\partial x}\right)^2 \ll \nu \frac{\partial^2 u}{\partial x^2}$$

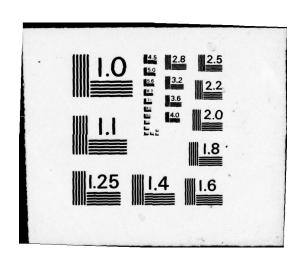
or dimensionally

$$\alpha^2 \frac{\Delta u \Delta x}{v} = \alpha^2 \operatorname{Re}_{\Delta x} << | \qquad (5.17)$$

With $Re_{\Delta x}$ generally larger than unity, the constant α must be chosen appreciably less than unity. This restricts severely the usefulness of the idea of using the artificial viscous term either for securing computational stability or for suppressing the shock induced oscillations in viscous flow problems.

For second order accurate conservative difference formulation, the errors introduced by the pseudo-viscous terms are included in the truncation error Em, the absolute upper bound of which may be estimated as $E_r < 3 \times 10^{-2} (Re_{\Lambda x})^2$ according to the results based on the Burgers' model equation given in the previous section. Thus $Re_{\Lambda x}$ may be as large as 1 or even 2 without having the cumulative truncation errors exceeding a few percent. Note that this Re Ax is defined in terms of the local change of velocity per mesh when the Burgers' model is applied to the "local flow field". With the Reynolds number based on the viscous flow dimension and maximum velocity of $0(10^3 - 10^4)$, and with possibly of $0(10^2)$ mesh points over the linear dimension, the local values of Re Ax will generally be considerably smaller than 10 (since Au per mesh will be significantly less than 10-1) except possibly in the region of shock induced oscillations. If the shock front is sisualized as an interior boundary and the shock-induced escillation as a form of propagating boundary error, the errors in the results computed with the second order accurate difference formulation will generally be dominated by boundary errors.





Shock induced oscillations mar the appearance of the computed solution much more seriously although need not cause larger error than the less conspicuous sources from the exterior boundary. The difficulty is compounded where a shock wave, either incident or emerging, intersects the exterior boundary. In the next section, the relation between the boundary treatment and the shock-induced oscillation will be explored.

5.4 Shock-Induced Oscillations

Shock induced oscillations are often considered as unavoidable when a shock wave is encountered in the computation with a higher order accurate difference algorithm. While the first order accurate algorithm will not give rise to such oscillations, the smear of the shock front becomes excessive and the cumulative truncation errors becomes large. Thus when shock wave is encountered in a computation, it is often held as necessary to choose between the two evils. The following is an attempt to clarify the origin of the spurious oscillations and to show that a certain class of second order accurate difference algorithms can, under some favorable circumstances, avoid such spurious shock-induced oscillations.

Consider the solution of a linear steady state problem via the time dependent approach. Let the spatial difference operator be split into two parts, $L_1(T)$ and $L_2(T)$ where T is the shift operator for the spatial indices, i.e., $TU_j = U_{j+1}$, $T^{-1}U_j = U_{j-1}$, and $T^2U_j = T \cdot TU_j = U_{j+2}$, etc. Construct the class of two step difference algorithms for the time interval $n\Delta t$ to $(n+1)\Delta t$:

$$\begin{cases} \tilde{U}_{j}^{n} - U_{j}^{n} = L_{1}(T)U_{j}^{n} + L_{2}(T)U_{j}^{n} \\ U_{j}^{n+1} - U_{j}^{n} = L_{1}(T)\tilde{U}_{j}^{n} + L_{2}(T)U_{j}^{n} \end{cases}$$
(5.18)

where \hat{U}_{j}^{n} is a provisional or predicated value of U_{j}^{n+1} and the second or final step is a corrector step. $L_{1}(T) + L_{2}(T)$ is second order accurate and consistent with the differential operator in the steady state.

Let the boundary conditions to be applied to the first or the provisional step be

$$B(T) \hat{U}_{i}^{n} = 0$$
 (5.19)

and let the boundary values of \tilde{U}_j^n , derived from these boundary conditions as are used in the first step, be used in the second step for the computation of U_j^{n+1} at the corresponding boundary points. In this manner it is maintained that $U_j^{n+1} - \tilde{U}_j^n \equiv 0$ on all the boundary points and at every time step. The boundary values at each boundary point may change from step to step and contain errors implicit in the boundary conditions (5.19). By subtracting the two steps in the difference equations (5.18) the following difference relation is obtained:

$$\left(U_{j}^{n+1}-\hat{U}_{j}^{n}\right)=L_{1}(T)\left(\hat{U}_{j}^{n}-U_{j}^{n}\right) \tag{5.20}$$

In the event that a steady state is approached in the sense that $U_j^{n+1} = U_j^n$, then Equation (5.20) becomes in the steady state limit

$$\left[1 + L_1(T)\right] \left(\tilde{U}_j^n - U_j^n\right) = 0 \tag{5.21}$$

Thus $\hat{U}^n_j - U^n_j$ is governed by the linear system of difference equations (5.21) and are subject to zero boundary values over the entire boundary. If there is no eigen solutions to this system of equations, it follows in the steady state limit that $U^n_j = \hat{U}^n_j = U^{n+1}_j$. Then the solution in the steady

state limit is the solution of the correct steady state equation

$$\left[L_{1}(T) + L_{2}(T)\right]U_{j}^{n} = 0 (5.22)$$

Now if the boundary values of \hat{U}_j^n and U_j^{n+1} are not kept the same in successive iterations, \hat{U}_j^n will have to be eliminated from Equations (5.18). Then, in the limit of the steady state with $\hat{U}_j^{n+1} = \hat{U}_j^n$, this solution will be determined by the equation

It will contain the "correct" steady state solution (5.22) to the extent that the boundary conditions $B(T)U_j^n=0$ represent the correctly posed situation. But it also contains the nontrivial solutions of Equation (5.21) when $\hat{U}_j^n-U_j^n$ is not identically zero, as a result of the slight difference in the boundary values of \hat{U}_j^n and U_j^{n+1} . Such extraneous solutions naturally are possible sources of the shock-induced oscillations and can indeed be identified in the course of computation as being proportional to the difference between the provisional and the final solutions. From the practical point of view, it is simpler and more desirable to use identical boundary values from (5.19) to suppress all the spurious fundamental solutions arising from Equation (5.21).

There are many two stap difference algorithms, but mostly not of the class (5.18) except the Cheng-Allen scheme and the Brailovskaya's scheme. For the linearized Burgers' Equation (3.13), the difference forms can be cast into: Cheng-Allen Algorithm [10,16]

$$\begin{cases} L_1(T) = \frac{1}{1+2s} \left[\left(-\frac{r}{2} + s \right) T + \left(\frac{r}{2} + s \right) T^{-1} \right] \\ L_2(T) = \frac{-2s}{1+2s} \end{cases}$$
 (5.24)

Brailovskaya Algorithm[17]

$$\begin{cases} L_1(T) = r(T - T^{-1}) \\ L_2(T) = s(T - 2 + T^{-1}) \end{cases}$$
 (5.25)

where $r = c\Delta t/\Delta x$ and $s = v\Delta t/\Delta x^2$. When (5.24) is substituted into Equation (5.23), the general solution of U_j is obtained as

$$U_j = \sum c_k \xi_k^j$$
 $k = 1, 2, 3, 4$

where

$$\begin{cases} \xi_1 = 1 \\ \xi_2 = \frac{2s+r}{2s-r} = \frac{1+\frac{1}{2} \operatorname{Re}_{\Delta x}}{1-\frac{1}{2} \operatorname{Re}_{\Delta x}} \end{cases}$$

snd
$$\xi_{3,4} = \left[-(1+2s) \pm \left\{ (1+2s)^2 + (r^2-s^2) \right\}^{1/2} \right] / (2s-r)$$
 (5.26)

 ξ_1^j and ξ_2^j are the two proper fundamental solutions of the correct steady state equation $[L_1(T) + L_2(T)]U_j = 0$, because in the limit of $Re_{\Delta x} + 0$, they approach the two fundamental solutions 1 and $\exp(Rex)$ of the steady state differential equation, $c_{\overline{\partial x}}^{\underline{\partial u}} = \frac{1}{Re} \frac{\partial^2 u}{\partial x^2}$. ξ_3^j , and ξ_4^j are the two extraneous fundamental solutions of the two-step scheme that constitute the errors or "spurious solutions" arising from the solution of the equation

$$\begin{bmatrix} \mathbf{I} + \mathbf{L}_1(\mathbf{T}) \end{bmatrix} \mathbf{U}_j = 0$$

or of Equation (5.21).

With both r and s > 0, and $\frac{|2s-r|}{2s+1}$ < 1, it is found that

$$\xi_3 \sim -\frac{r+2s}{1+2s} < 0$$

$$\xi_4 \sim -\frac{(1+2s)}{2s-r} \stackrel{>}{\sim} 0 \text{ as } r \stackrel{>}{\sim} 2s.$$

Thus ξ_3^j always represents mesh to mesh oscillation while ξ_4^j can be either oscillatory or monotomic. The steady state limit of the difference $U^{n+1} - \hat{U}^n$ can be given as:

$$\tilde{V}_{j} - V_{j} = c_{3}\xi_{3}^{j} + c_{4}\xi_{4}^{j}$$
 (5.27)

where c_3 and c_4 are determined by the difference in the boundary values of U^n and U^{n+1} at j=0 and j=J on the boundary. When the boundary values of U^n and U^{n+1} are kept the same at every step, then $c_3=c_4=0$ and no spurious solution will be present in the computed steady state result. Otherwise, oscillations can be expected in the computed steady state result.

If Brailovskaya's scheme (5.25) is substituted into Equation (5.23), the same proper fundamental solutions $\xi_1^{\ j}$ and $\xi_2^{\ j}$ are obtained, but the pair of extraneous solutions $\xi_3^{\ j}$ and $\xi_4^{\ j}$ are given somewhat differently with $\xi_{3,4} = \left[1 \pm (1 + 4r^2)^{1/2}\right]/2r$, and $\xi_4 < 0$ always. The overall situation is much the same.

It may be pertinent to repeat here that the spurious solutions will be suppressed so long as the same boundary values of \hat{U}^n and U^{n+1} are used at every step. Such boundary values can be determined by the approximate boundary conditions $B(T)U_j^n=0$, and may contain errors. In this event, they may cause errors in the constants c_1 and c_2 of the steady state

solution

$$U_{j} = c_{1}\xi_{1}^{j} + c_{2}\xi_{2}^{j} \tag{5.28}$$

There will not be any catastrophe if the boundary values are not excessively in error and if the mesh size of the steady state solution is not too coarse so that

$$Re_{\Delta x} < 2$$
 (5.29)

This last restriction $\operatorname{Re}_{\Delta x} < 2$ has little to do with suppressing the spurious fundamental solution, ξ_3^j and ξ_4^j . It is to keep ξ_2^j from being oscillatory and failing to be a valid approximation to the fundamental solution $\exp \left|\operatorname{Rej}\Delta x\right|$ of the differential problem. It is clear from Equation (5.26) that when $\operatorname{Re}_{\Delta x} > 2$, the appropriate form of ξ_2^j is

$$\xi_2^{j} = (-1)^{j} \left[\frac{1 + 2/\text{Re}_{\Delta x}}{1 - 2/\text{re}_{\Delta x}} \right]^{j}$$
 (5.29)

which is oscillatory and rapidly amplifying with increasing j. It fails to serve as any meaningful approximation to exp $|\text{Rej}\Delta x|$. Thus to obtain a valid steady state solution without spurious oscillations based on the algorithms (5.24) or (5.25), not only that identical boundary values should be used at the provisional and the final steps, but also that the mosh size must be sufficiently refined so that $\text{Re}_{\Delta x} < 2$. Sample calculations for the steady state solutions of the linearized Burgers' equation (3.13) verified the abrupt change of the behavior from a smooth to a violently oscillatory limiting solution when $\text{Re}_{\Delta x}$ increases beyond the critical value of 2.

For linear problems with variable coefficients, the various fundamental solutions of the difference equations cannot be displayed. It is nevertheless expected that the spurious solutions will be suppressed if the same operators L, (T) and L, (T) and the same boundary values are used for the successive iterative steps in every time interval. As to the proper fundamental solutions of $[L_1(T) + L_2(T)]U_i = 0$, it is known that one of them must be unity because of the consistency requirement. The other will become oscillatory for too large a ReAx. Whether the critical value of $Re_{\Lambda x}$ will be 2 or how it may vary with x is uncertain. For nonlinear problems with sufficiently smooth solutions, the complete suppression of the spurious fundamental solutions in the first variation of the nonlinear difference operator at each time step, may be expected. This is because the spurious fundamental solutions contained in the computed results of the nonlinear equations will have been reduced to higher order small quantities in Δt by the stratagem described above. Such higher order small quantities in At will be of little significance in the steady state limit. Thus, the outstanding problem for eliminating shockinduced oscillations is to satisfy the requirement of using some sufficiently small mesh size Δx corresponding to the restriction of $Re_{\Delta x} < 2$ for the linearized Burgers' equation. It is anticipated that, for nonlinear problems, there may not be such a sharp value of the critical Rear. The transition from smooth to oscillatory steady state solution may be gradual over some range of values of Re Ax. This has also been verified with actual computation. It is supposed that the following heuristic model will give a general idea where this critical range of Reax may be.

When a second order accurate conservative difference algorithms of the class (5.18) is used for the integration of the Navier-Stokes equations and when the stratagem, just described, is followed in the treatment of the boundary conditions, the shock wave, if present in the computation, is not regarded as a discontinuity but a "smooth" region with large gradient, spread out by the pseudo-viscosity. This shock transition region usually spreads out over two or more mesh points to connect the smooth, asymptotically uniform flow fields both up and downstream of the shock region. The transition profile as calculated is not intended to be accurate. Its primary function is to accomplish a smooth connection, and hopefully, without inducing oscillations propagating into the smooth flow field in its neighborhood. Thus, transition profile joining a scalar function u with asymptotic values u = ± a in the up and the downstream region respectively, might as well be computed approximately based on the nonlinear Burgers' equation as a model for the local flow field .. This means that the local profile might be approximated by the steady solution, Equation (5.10) with x = 0 and u = 0 located at the point of maximum slope in the transition profile that has been actually computed with the full Navier-Stokes equations. Thus, the computed maximum value of $\frac{\partial u}{\partial x}$ properly nondimensionalized in the transition region will define the effective Reynolds number of the transition region.

$$\left(\frac{\partial u}{\partial x}\right)_{\text{max computed}} = \text{Re}/2$$
 (5.30)

In this manner, the poorly defined thickness of the transition region is avoided. The parameter a can be taken as unity when the reference velocity is adopted as the change of the velocity (or the particular scalar quantity in dimensionless form) from the point of maximum gradient to the asymptotic value. If the computed transition profile is approximately symmetric with respect to the inflexion point, this reference velocity will be half the jump across the shock.

Let the asymptotic values of u across the shock transition region be U_1 and U_2 then, assuming $U_1 > U_2$,

$$\left(\frac{\partial U}{\partial x}\right)_{\max} = \frac{U_{1} - U_{2}}{2} \left(\frac{\partial u}{\partial x}\right)_{\max} = \frac{U_{1} - U_{2}}{4} \operatorname{Re}$$

$$\left(\Delta U\right)_{\max} = \left(\frac{\partial U}{\partial x}\right)_{\max} \Delta x = \frac{U_{1} - U_{2}}{4} \operatorname{Re}_{\Delta x} \tag{5.31}$$

Now it is pressumed that the critical value of this $Re_{\Delta x}$ is essentially the same as if the computation were done with the same algorithm but based on the Burgers' equation so that oscillation-free computed results of the transition region can be effected with $Re_{\Delta x} < 2$. When expressed in terms of quantities, directly available in the computation as an a posteriori criterion, according to (5.31), this condition becomes

$$\frac{(\Delta U)_{\text{max}}}{U_1 - U_2} < \frac{1}{2} \tag{5.32}$$

i.e., "the maximum permissible change of U per mesh $(\Delta U)_{max}$ is one half the jump $|U_1-U_2|$ across the discontinuity so as to avoid shock-induced large oscillations in the computed results."

This statement implies that we cannot expect to obtain an oscillation-free shock front that contains less than two meshes from the computational solution following the present stratagem. Moreover, within the linearized framework, the criterion (5.32) should be equally applicable to any physical scalar variable, sustaining a "jump" across some large gradient region not necessarily a discontinuous front, although the $\text{Re}_{\Delta x}$ was defined in terms of flow velocity and viscosity. It is independent of viscosity explicitly.

The criterion (5.32) stands, however, only as an a posteriori criterion for achieving an oscillation-free shock solution. This is because $(\Delta U)_{max} = \left(\frac{\partial U}{\partial x}\right)_{max} \Delta x$ becomes known only after the completion of the computations; by then, there is no need of the criterion to find out if the computed solution is oscillation-free! Such an a posteriori criterion can, however, be of some help in practice, since $(\Delta U)_{max}$ can be estimated long before the computed solutions reaches a satisfactory "steady state". Oscillations will be present in the "transient states" of the computation whether or not the steady state limit will contain shock-induced oscillations. If the criterion should be satisfied at some transient stage, we may expect an oscillation-free steady state solution with further temporal steps. Otherwise, smaller mesh sizes may be needed.

It is more convenient if this criterion can be put into some a priori form, less precise as it must be. Note that the magnitude $|U_1-U_2|$ depends on the shock strength, the shock orientation relative to the coordinate axes (in a multi-dimensional problem) and the coordinate direction under consideration. If it is possible to estimate this magnitude $|U_1-U_2|$, then

$$Re_{\Delta x} \stackrel{\sim}{=} |U_1 - U_2| \Delta x/2v < 2$$

may be used directly as an a priori limit. This Reynolds number $\text{Re}_{\Delta x}$ must not be confused with the $\text{Re}_{\Delta x, \infty}$ based on the uniform supersonic flow velocity U_{∞} far upstream of the flow field, i.e., $\text{Re}_{\Delta x, \infty} = \text{U}_{\infty} \Delta x / \nu$. In

terms of this $Re_{\Delta x, \infty}$, the criterion becomes

$$Re_{\Delta x,\infty} = \frac{U_{\infty}\Delta x}{v} < \frac{U_{\infty}}{U_{1}} = \frac{4}{1 - U_{2}/U_{1}}$$
 (5.33)

which can be useful apriori if there is some idea as to the shock strength U_2/U_1 and the ratio U_∞/U_1 of the reference velocity U_∞ far upstream to the velocity U_1 into which the shock wave is propagating. For complicated flow problems, however, such quantities are usually among the unknowns. Thus, the limit on $\operatorname{Re}_{\Delta x,\infty}$ given by (5.33) will have to be based on some rough estimate or on the "transient states" of the computed solution.

The previous heuristic development is equally applicable to any flow region containing large gradients other than the shock front. In particular, oscillations originating from boundaries of the field of computation can be likewise alleviated. It is to be emphasized, however, that if the oscillatory extraneous fundamental solutions like ξ_3^j and ξ_4^j were not suppressed by the stratagem described above, these extraneous oscillatory solutions will propagate into the neighboring smooth flow fields even if the mesh size is much reduced below what is required by (5.33), at least one of them will be amplifying away from the boundaries of the transition region while propagating into the neighboring smooth regions on either side. On the other hand, if much too coarse a mesh size is used in the computation, large amplitude oscillations will result since one of the proper fundamental solutions of the difference equation fails to be a valid approximation to that of the differential problem despite the fact that the stratagem described above is followed. To produce an oscillation-free computational solution of a flow problem involving shock waves, it is recommended not only that some form of the two step algorithm (5.18) be used with identical boundary values applied to both iterative steps during a

time interval, but also that the mesh size Δx is kept sufficiently small compared with the condition (5.33). This recommendation is based on the results of analysis of a simple model linear equation for the numerical solution of the much more complicated and nonlinear gas dynamic equations. It is recommended in the same spirit that the local, linear stability analysis of v.Neumann will help in achieving computational stability. The practical merit of this recommendation is yet to be examined in greater detail by the computational community.

The previous development has guided the author quite successfully in his earlier attempts of integrations of the Navier-Stokes equations for some complicated flow problems, such as the near wake flow behind a flat base with a sharp corner in a supersonic flow and the hypersonic flow over the sharp leading edge of a highly cooled flat plate. The flow situations encountered in these examples are just too complicated to provide any meaningful quantitative tests of the validity of this criterion and the accuracy of the computed results. In the following a simple case will be described which may serve to support and to illustrate the usefulness of the stratagem and the simple criterion despite the heuristic content of its application to the actual integration of the Navier-Stokes equations.

The Cheng-Allen two step algorithm as a member of the class (5.18) is used to integrate the complete Navier-Stokes equations for the propagation of a planar shock wave into a uniform supersonic flow at Mach No. 2 with the shock front inclined at an angle $\beta = 41.84^{\circ}$ to the uniform in[19]
flow. The gas density ρ_1 , velocity u_1 , energy e_1 , and pressure p_1 are taken to be unity in dimensionless form. The theoretical values of these variables downstream of the shock, according to the Hugoniot relations agree

with the values computed at $\text{Re}_{\Delta x,\infty} = 10$ to better than 0.1%. The critical Reynolds number per mesh is $(\text{Re}_{\Delta x,\infty})_c = 4/(1-0.837) = 24.5$. No oscillations are found. The shock front is sharp and straight. It is verified that the a posteriori criteria (5.32) are satisfied for the density ρ the x-velocity component u, the y-velocity component v, the energy e and the pressure p across the shock.

When the computation is repeated at ${\rm Re}_{\Delta x,\infty}=50$ exceeding the critical value $({\rm Re}_{\Delta x,\infty})_{\rm C}=24.5$ for the same flow configuration, substantial oscillations are present immediately downstream of the shock. The a posteriori criteria (5.32) for all the physical variables are found violated. The peak amplitude of the oscillation is about 10% but such oscillations are essentially damped out a few meshes downstream of the shock. The downstream asymptotic values are reached well within the field of computation. The downstream asymptotic values obtained from the computation at ${\rm Re}_{\Delta x,\infty}=50$ are correct to within 0.3% of the Hugoniot values.

The smooth incident shock computed at $\text{Re}_{\Delta x,\infty}=10$ was then allowed to be reflected from an inviscid wall. For the reflected shock, the critical Reynolds number $(\text{Re}_{\Delta x,\infty})_{\text{C}}=4/(0.837-0.646)=21$, which exceeds the $\text{Re}_{\Delta x,\infty}=10$ used in the computation. A smooth, straight reflected shock is obtained. All the computed downstream appropriate values agree with the theoretical values to better than 0.1% and there are no oscillations.

Computations at intermediate values of $Re_{\Delta X}$ indicate that oscillations begin to appear with $Re_{\Delta X}$ exceeding 10 to 15, increase most rapidly around the critical value of 20 - 30, and keep increasing slowly with larger $Re_{\Delta X}$. This gradual rather than an abrupt change of behavior with

Reax is probably what should be expected in a nonlinear system. It is encouraging that the simple criterion obtained from an elementary linear analysis of a simple model may prove to be useful in complicated flow problems to be encountered in practice.

VI. CURRENT STATUS AND FUTURE PROSPECT

The various problems associated with the numerical integration of Navier-Stokes equations have been reviewed in the previous chapters as to the mathematical origin of the problems and of the basis of various techniques in dealing with them. This approach was chosen in preference to a review in the form of a glossary of various solutions in the literature so as to provide a frame of reference how such solutions may be studied and how each specific problem should be approached.

In the days of the mechanical desk calculators or the card programmed calculators (CPC), the numerical integration of the hydrodynamic equations was attempted. The primary concern then was the limitation of the computational speed offered by these mechines. While the question of computational stability was known to mathematicians, it is not of much concern to the practitioners. The dawn of the high speed electronic computers in the mid-1940's changed all that. The ability to compute fast showed how often an apparently straightforward computation will lead to unbounded meaningless results. This problem is the first and the most pressing one presented by the high speed computers. If the stability question of the computation is not successfully resolved, no results of any kind could be obtained. Since the mid 1940's, this stability question has been studied very extensively, both mathematically and empirically. As was described in Chapter III, much has been learned and understood since

then. It is still true that when complicated sets of partial differential equations such as those of gas dynamics are to be integrated, computational stability remains a formidable problem. As in the older days, so much work is still needed to render a stable computation that one often hesitates to ask any further questions about any reasonably looking computed solution. But for those interested in computational methods for some practical purposes, computational stability is not synonymous with the major problem of the computational solution of a partial differential equation system. It is only a first step in achieving a solution of value in practice.

With the help of suitable model studies and appropriate choices of difference algorithms, computational stability can generally be obtained and tested in actual machine computation. Now is the time to be concerned with obtaining not only some qualitatively correct solutions but also quantitatively correct answers with some estimate of the error bounds of the computed solution. In applications, the primary purpose of a computed solution is to seek some reasonably accurate quantitative estimate of the flow field. The accuracy requirements for different applications may be quite different. Whether a solution is sufficiently accurate for a specific application can only be judged under some overall view. But such a judgement can be made only when the computed solution is accompanied by an error bound if not a strict error estimate. The error bounds of a computed solution is no less important than the error bars of a set of experimental data if such computed or experimental sets of data are to be practically useful. With this in view, the preliminary developments on computational accuracy given in Chapters IV and V are very important

in practice. Most of the solutions available in published literature cannot be examined with regard to the question of accuracy because they were probably obtained primarily to demonstrate qualitatively what can be doen rather than to solve specific problems in application. A few examples will be described below with some comment.

6.1 Hydrodynamics

The flow of an incompressible viscous fluid in two space dimension probably represents the simplest form of the Navier-Stokes equations. It is most often treated in the stream-function-vorticity form. The mass continuity equation in two space dimension (x,y)

$$\frac{\partial \mathbf{u}}{\partial \mathbf{x}} + \frac{\partial \mathbf{v}}{\partial \mathbf{y}} = 0 \tag{6.1}$$

can be satisfied by a scalar stream function Y defined with

$$u = \frac{\partial \Psi}{\partial y}$$
 and $v = -\frac{\partial \Psi}{\partial x}$ (6.2)

while the vorticity component ω normal to the x-y surface is

$$\nabla^2 \Psi = \frac{\partial^2 \Psi}{\partial x^2} + \frac{\partial^2 \Psi}{\partial y^2} = -\omega(x,y) \tag{6.3}$$

The curl of the momentum equation reduces to the vorticity transport equation

$$\frac{\partial \omega}{\partial t} + \frac{\partial \Psi}{\partial y} \frac{\partial \omega}{\partial x} - \frac{\partial \Psi}{\partial x} \cdot \frac{\partial \omega}{\partial y} = v \nabla^2 \omega \tag{6.4}$$

The divergence of the momentum equation gives the $\nabla^2 p$ in terms of Ψ and ω . Thus the static pressure in the flow field can be solved independently after the stream function Ψ and vorticity ω have been determined. Thus

the solution for a hydrodynamic problem will be posed as the solution for two elliptic problems for Ψ and ω simultaneously represented by Equations (6.3) and (6.4) subject to Dirichelet and/or Neumann boundary conditions on a closed boundary for Ψ and ω . The physical boundary condition depends on the problem.

A simplest case is the decay of a vortex in a closed rectangular box in which case u = v = 0 on the boundary which may be taken as x = 0, y = 0, x = 1, y = 1, respectively. This set of physical boundary conditions has to be translated into boundary conditions of Ψ and ω . By definition $\Psi = 0$ may be assigned on the boundary. This serves to determine $\Psi(x,y)$ completely from (6.3) when $\omega(x,y)$ is given over the field. The remaining physical boundary conditions are

$$\frac{\partial \Psi}{\partial y} = u = 0 \quad \text{on} \quad x = 0 \quad \text{or} \quad x = 1$$

$$-\frac{\partial \Psi}{\partial x} = v = 0 \quad \text{on} \quad y = 0 \quad \text{or} \quad y = 1 \quad (6.5)$$

The practical question arises how (6.5) may be expressed as the boundary conditions of ω in the solution of Equation (6.4). In practice, this question is by-passed by solving Equation (6.3) first for the advanced values of $\Psi(x,y)$ and the boundary values of ω are estimated either from the initial data or the results of the most recently available advanced values of Ψ near the boundary. This can be done either with or without the conditions (6.5) taken into consideration. In principle the boundary conditions (6.5) should at least be checked a posteriori. There is clearly an error τ_B on the boundary values of ω of the order of Δt , Δx , and/or Δy depending on the formal order of accuracy how this boundary condition is handled.

Now if Equation (6.4) is integrated over the volume (i.e., x = 0 to 1 and y = 0 to 1) and over the time period t = 0 to t of the integration, the total decay of the vorticity is

$$\int_{V} [\omega_{0}(t = 0) - \omega(t)] dV$$

$$= v \int_{0}^{t} dt \int_{V} \nabla^{2} \omega dV$$

$$= v \int_{0}^{t} dt \int_{s} (\vec{\nabla} \cdot \omega) \cdot d\vec{n}$$
(6.6)

i.e., proportional to the total outflux of the gradient of vorticity on the boundary. (The three dimensional analog is obvious). Thus the nonrandom cumulative error on the total decay of the vorticity in the box will be of the order of $NJ\tau_{\rm R}$ where N is the number of time steps integrated and J is the number of spatial meshes in a linear dimension. The \vec{v} · ω on the boundary is assumed to be of the same order as the error in the boundary vorticity τ_R itself. The use of the integral formula implies that the accumulation of the truncation errors over all the interior points have been neglected in the difference formulation. Even so, the total dacay of the vorticity at later times depend very importantly on how accurately the boundary vorticity was formulated in the computation and on whether and how the errors associated with such a formulation will accumulate in space (along the boundary) and in time. The question is more than the local truncation error of the difference formulation of the vorticity boundary condition since the correct physical boundary condition Equation (6.5), which represents some integrated condition on the vortcity field rather than the local values of the vorticity was ignored.

The use of the stream function-vorticity as the dependent variables is the fundamental reason of the difficulty in implementing the boundary

conservative formulation to prevent the accumulation of the truncation errors over the interior points. If the physical variables u and v are used as the dependent variable in the difference formulation, the difficulty with the boundary condition would be eliminated for the above example and the conservation of the difference formulation can be readily implemented. The advantage of the vorticity-stream function formulation in reducing the number of partial differential equations may be more than compensated by the difficulty it brings for this problem.

For hydrodynamic problems with inflow and outflow boundary in the field of computation, the boundary treatment in the difference formulation faces a difficulty of different nature. This is because the physical boundary conditions are prescribed very far up and downstream of the field of computation. The vorticity-stream function formulation does not aggravate the situation much further and is therefore often preferred for the numerical integration of the hydrodynamic equations. The Poisson type equations can be efficiently solved in different ways. There are many such solutions in the literature. Most of such results can not be analyzed for an error estimate primarily because of the non-conservative form of the difference formulation that permits the accumulation of the local truncation errors. Experimental data are generally not available to provide a quantitative estimate of the error of the computed results. All such computations serve to demonstrate the feasibility of computing some "reasonable" approximate solutions but are of little quantitative value. A numerical study of the steady flow of a uniform stream over a sphere was therefore undertaken by Rimon and Cheng.

The flow field of a uniform stream over a sphere is conveniently described by using the spherical polar coordinates. To extend the outer boundary of the field of computation to as far downstream as possible to facilitate the implementation of the boundary conditions, $z = \ln r$ is used in place of the physical radius r. Three different sets of numerical integration have been made by different authors at common Reynolds numbers of 40 and 100. There is also a set of experimental data by Taneda [23] of some characteristic quantities of the recirculatory wake flow field at these and other Reynolds numbers. Such measured values of wake length, locations of the separation point and the vorticity centers provide comparisons of the detailed flow field in the most sensitive region, in addition to the overall drag coefficient acting on the sphere.

Jenson and Hamielec, et al. used similar difference relaxation procedures and used the same downstream boundary conditions approximating uniform out flow. Both cases were carefully executed and examined numerically, very carefully, and made sure that the steady state results they obtained are essentially independent of further reduction of mesh spacing from mesh sizes $\Delta\theta = 6^{\circ}$ and z = 1/20. They obtained the same drag coefficient C_D in agreement with what is expected from the experimentally well-established standard drag curve. However, the details of the two solutions were much different. For example, the vorticity on the wake side of sphere surface differ by a factor of 2 to 3 for the case with $Re_D = 40$. The streamline patterns in the recirculatory wake are visibly different although qualitatively similar. It is supposed that such differences in the results largely demonstrate the cumulative effects of the truncation errors due to the non-conservative nature of the difference

algorithms equivalent to their relaxation procedures. Jenson's results depart considerably further from Taneda's wake data than the results of Hamielec, at al. at Re_D = 40. Hamielec, et al. also calculated the case Re_D = 100. They found it necessary to refine the mesh to $\Delta\theta$ = 3° and Δz = 1/40 to secure a reasonable steady state and to introduce some fine adjustments in order to reproduce the experimental value of the drag coefficient C_D at Re_D = 100.

Rimon and Cheng succeeded in developing a conservative difference form that is still reasonably simple despite the contracted curvilinear coordinates and stream function vorticity formulation. The same mesh size $\Delta\theta = 6^{\circ}$ and $\Delta z = 1/20$, as was used by the previous authors, was used. The conservative nature of the difference formulation permit an estimate of the upper bound of the cumulated truncation error by Equation (5.14). The Re_{Λ_X} should be replaced by Re_{Λ_Z} for this calculation in terms of $\Delta\theta$ and Δz . The magnitudes of $Re_{\Delta z}$ for the two cases with Re_D = 40 and 100 can be estimated from the computed solution based upon the velocity gradient in the region near the isolated rear stagnation point in the wake (the reference velocity of this mesh Reynolds number is based on the velocity difference across the large gradient region). They are less than $\frac{1}{2}$ and 1 respectively. Accordingly, the absolute upper bound of the cumulated truncation errors are $3 \times 10^{-2} \times \text{Re}_{\Delta z}^{2} \sim 1$ and 3% respectively. The extrapolation condition at the downstream boundary gives rise to the largest contribution to the boundary error, Both $\frac{\partial \Psi}{\partial x} = 0$ and $\omega = 0$ on the out flow boundary may commit a fractional error as much as 100%. (It is not expected to error in sign). The absolute upper bound of the boundary errors may then be estimated with Equation (5.16) where $\varepsilon_h = 1$ and Re is based on the maximum flow velocity in the wake region and the

length from the rear stagnation point to the out flow boundary in the z- θ plane of computation. This is more than two unit lengths. The effective Reynolds numbers are then 80 and 200 respectively. Accordingly, the bounds of the boundary errors are estimated as $2\varepsilon_b^*/Re$ of 2.5% and 1% respectively. By adding the estimates of the absolute upper bounds of the truncation errors and the boundary errors for each case, the overall estimate of the absolute error bounds are about 3.5% and 4% for the cases $Re_D = 40$ and 100 respectively. This is a quite satisfactory engineering accuracy. Thus, it is expected and verified that the computed results of Rimon and Cheng will agree with Taneda's wake data much better than the results of Jenson and Hamielec, et al. The computed vorticity field in the near wake region of Rimon and Cheng and that from Hamielec, et al. differ by a factor of 2 or more in the case with $Re_D = 100$ while they differ much less for the case $Re_D = 40$. This again demonstrates the significance of the accumulation of the local truncation errors.

The computational effort of the solution of this problem following the formulation of Rimon and Chengwas not excessive at the time and is rather small in terms of the present day computing machines. 61 × 31 = 1891 mesh points were used. Steady state solution was obtained in about an hour computation per case in the IBM 7094, with the potential flow as the initial data. In terms of CDC 6600 machine time, it would take less than 10 minutes. The computational time can be appreciably reduced if a more reasonable approximation than the inviscid flow field should be used as the initial data. It is therefore believed that with conscientious effort in constructing the difference formulation, useful quantitative results can be obtained from the numerical solution of the Navier-Stokes equations.

The extension of such calculations to steady flows in three dimensional space and to higher flow Reynolds numbers will need not only substantially more computer time but also some analysis to gain understanding of certain intricacies in the 3-D problems especially concerning the computations in the vicinity of "separation lines". With the greatly increased capability of the high speed computers in the foreseeable future, it is reasonable to expect good quantitative results for these steady 3-D problems of practical interest.

The time dependent hydrodynamic problems in three space dimensions may be considerably more difficult and demanding. This is especially true if the hydrodynamic turbulence is the subject of investigation. The high frequency components of the turbulent fluctuations could doubtfully be treated with a reasonable accuracy despite the giant stride in the capability of the computing machines foreseen in the future. It appears that some phenomenological theory, at least for the high frequency components, will be needed while the low frequency components may be satisfactorily handled by computational methods. This statement is meant to apply whether it is to be integrated in the physical space with the physical variables or it is to be treated in the Fourier space for the Fourier components of the physical variables. Much work is needed in any case [24,25,26]

6.2 Supersonic Gas Dynamics

The gas dynamic equations system is basically the same as the hydrodynamic equations except for the variations of gas density and the diffusivities and for the addition of the equation of energy balance (1.3). The outstanding feature of the supersonic flow field is the presence of shock waves either generated from within or incident on the flow field from without. Most of the practical problems that call for the numerical treatment of the Navier Stokes equations involve the generation of shock wave from the interaction between the inviscid and the viscous streams. The computation of a shock wave with unknown strength and location presents considerable difficulties as was discussed in the previous chapter. The shock-induced oscillations in its neighboring flow field is detrimental to the appearance of the computational solution. Such solutions were often presented after some artificial averaging or filtering procedure and can, therefore, be of qualitative values only. Those solutions relatively free from this criticism indeed two their success in avoiding the serious consequences of a shock standing in an important part of the flow field. By carefully selecting the field of computation for the problems to be investigated, they minimized the consequences of shock-induced oscillations.

Allen and Cheng treated the near wake flow inbedded in a supersonic stream turning over a sharp shoulder with a "recompression shock" generated from the turning of the supersonic stream caused by the closing of the recirculatory wake. In the steady state solution of this problem, the small oscillations caused by the recompression shock distorts appreciably the computed results only in the far downstream portion of the rejoined wake flow field near the downstream boundary. Although the oscillations of the flow properties in the flow field is equivalent to those induced by an oscillation of the shock front of only $1/4\Delta x$, it remains as one of the two largest sources of computational errors. It is conjectured that the likely source of the small oscillation is the extraneous inaccurate difference treatment where the shock emerges from the downstream boundary

of the field of computations. The conservative difference form of the class (5.18) was used and the criterion (5.33) is satisfied although without a substantial margin. Unfortunately, comparable experimental data are not available and the extension of this calculation to the range of practical Reynclds numbers of 10^3 - 10^4 and for the somewhat more complicated geometrical configuration was beyond the means (cost of computations) available.

[27]
Ross and Cheng studied the question that if the number of mesh points is limited to 2100 with "optimal" ratio of $\Delta x/\Delta y$ and with some non-essential but simplifying modifications of the boundary treatment, what the range of the Reynolds numbers and Mach numbers will be when the computational solutions with the previous formulation will possess an absolute upper bound of the error of no more than 10%. The computational effort was limited to 10-15 minutes of computing time on the IBM 360-91 equivalent roughly to 20-30 minutes on the CDC 6600 or 4 to 10 hours on the IBM 7044, originally used by Allen. When other restrictions purely of fluid mechanical nature are superposed, it was established that the range of validity of the computational formulation can be extended to M = 4 and Reynolds numbers of ~ 1-2 × 103 based on half width of the base. To extend this computation to the practical range of interest would require substantial refinement in the mesh size with corresponding increase of the computational effort. The storage requirement on the computer does not seem restrictive. It was the computer time and cost that was prohibitive. It may be that the absolute upper bound of 10% is too restrictive since the maximum fractional error in the solution is likely to be substantially less than the absolute upper bound. A substantial decrease of the estimate of the computational effort will follow a modest reduction of the accuracy requirement if the

mothod of error estimate described in Chapter V should be granted in the absence of any direct comparison with reliable and comparable experimental data.

[28]
Carter chooses to integrate the Navier-Stokes equation for a steady supersonic viscous flow over a compression ramp or corner with an imbedded separated region. The compression waves will eventially coalesce into a shock wave. Carter kept the upper boundary of the field of computation sufficiently close to the viscous region so that the waves generated from the viscous layer may be treated as isentropic waves without serious error and utilized the simple wave extrapolation condition on the upper boundary. This stratagem, as was used in the treatment of the near wake problem. serves to eliminate the major part of the undesirable wave reflection from the upper boundary. By restricting the field of computation to such a narrow strip and using a highly refined mesh with Brailovskaya's difference algorithm, a member of the class of (5.18), the results compare favorably with experimental data in the comparable Reynolds and Mach number ranges. The difference formulation is probably not quite conservative due to the use of the "curved" body coordinates. But the curvature is sufficiently small or otherwise localized so that the accumulation of the truncation errors may not be excessive. While an estimate of the error bounds has not yet been made, the evidence seems to indicate that this calculation may have come very close to generating directly some useful practical results. Admittedly, the computational effort in this calculation seemed to be excessive from the academic point of view, (two or more hours of CDC 6600 per case), it does not appear prohibitive from the view of engineering development. Moreover, there is substantial room for improvements if an error estimate can be made. The 4th generation computers that will

shortly be operational further promise a substantial increase in speed of computations and in storage capability. This may render the computational effort to be of less concern in solving such practical problems.

An academic program has been devoted to developing techniques to face the difficulty of computing shock waves in a complicated flow field. The results reported in Section 5.4 demonstrated some progress in this direction. There are still tremendous difficulties ahead and, as yet, not resolved when the shock wave interacts with other incident waves and when the criterion of (5.33) becomes much too restrictive. Nevertheless, even in the present unsatisfactory state, the computational results can be useful in fluid dynamics research to supplement experimental and other efforts. They will also encounter difficulties, but of some different nature. The following treatment of the hypersonic leading edge problem may illustrate the situation.

Over the leading edge of an infinitely thin flat plate, placed in a hypersonic or supersonic stream at zero incidence, a shock wave will develop due to the viscous effects in the vicinity of the plate. In this region, the hypersonic strong interaction theory, based on the boundary layer type arguments, failed to provide even a qualitatively adequate description of the flow field. It is in doubt to what extent the flow situation will have to be described by the kinetic theory rather than by the continuum theory when appropriately modified for the slip effects. The flow field was thus computed by Chen and Cheng. A rather strong oblique shock wave develops rapidly from the leading edge, and produces, in the downstream gas, a high pressure and temperature, both proportional to M²sin²θ where θ is the local inclination of the shock front with the incoming uniform stream. It is very clear then that any small oscillations

in the shock front will produce, in the downstream, corresponding oscillations of very significant magnitudes with the upstream flow Mach number of ~ 20. It is, therefore, very critical to have the shock oscillations essentially eliminated from the computation. The conservative two step algorithm of Cheng and Allen was again used with a 40 × 30 mesh in the physical space x-y with y = 0 describing the plate surface. The leading edge shock emerges from the downstream out flow foundary just below the top corner. No oscillation of the shock wave is noted except in the immediate vicinity of the plate leading edge point. The oscillation is fairly large but dies out rapidly within about 5 meshes downstream along the plate and 2-3 meshes normal to the plate. Various slip conditions were used in the computation. A minor localized oscillation developed somewhere downstream about 2-4 by for no obvious reasons and is far away from the shock. It is conjectured to have originated from some inappropriate treatment of the boundary conditions on the plate. This localized oscillation imposes no significant error on the solution. The downstream out flow boundary is again treated by the second order accurate extrapolation but along the shock direction where the shock emerges, along the plate on the plate surface and along directions linearly interpolated in between. Despite the suppression of the oscillations of the emerging shock, the slow decay of this boundary error stands as the largest single contributor to the solution in the interior. The absolute upper bound is <7% according to Equation (5.16) as evaluated with the smooth computed solution a posteriori. The truncation error as evaluated with Equation (5.14) and the solution in the non-oscillatory region away from the leading edge point is less than 78. With both the round-off error and the error

due to the steady state criterion both less than 1%, it is estimated that the absolute upper bound of the error in the computed solution, away from the immediate vicinity of the leading edge and the out flow boundary, is 16%. The scatter of experimental data is more than 50%.

Comparison of the computed results with a collection of experimental data, not precisely corresponding but encompassing the case computed, shows substantial agreement with the data considered to be most reliable in the different regions and for different quantities. This comparison is certainly not the best and the most definitive, but is probably the best available and possibly the best one may hope to have in the not too distant future. This is in view of the difficulty in reproducing the experimental environments and of the cost involved in such experiments. This study leads to a few physically meaningful conclusions which was not possible otherwise. They are

- (1) A continuum formulation with appropriate slip condition is physically plausible and can indeed be useful for prediction purposes probably more reliable than experiments.
- (2) The surface conditions based on totally diffused reflection and zero recovery of mean kinetic energy is the only correct one that can provide the low surface pressure in the range of the available experimental data.
- (3) The computational method with a reasonable accuracy can be useful in fluid dynamics research and can help to resolve difficult fundamental problems. It is not simply a tool for carrying out repetitive routine numerical work in engineering development.

There are important omissions, in the above review, of many interesting and significant results in the development of computational methods relevant to aerospace applications. They are omitted here to facilitate the presentation of the major theme and hopefully with as little digression as possible. While computational stability remains a problem, it can generally be overcome with some hard work. It should not be permitted to draw attention away from the need of reasonably accurate computed results. Stable and smooth computational results are encouraging but can be very deceiving. From the application point of view, the question of accuracy is crucial. Accordingly, the approach described above to secure "accurate" formulation is of fundamental importance, crude as it is. How such crude criteria may be used and incorporated are desmonstrated in this chapter. Much development in this direction is needed. Some fundamental aspects should be understood and practical methods developed to deal with the various situations. Such problems will not fade away because of the dramatic advance in computer capabilities. Indeed, there are serious problems that will be encountered in the efficient use of the fourth generation computers if any meaningful speed advantages are to be reaped. Therefore, a few words on the prospects of the coming fourth generation computer will serve to bring to conclusion the present review.

6.3 Future Prospects with the Fourth Generation Computers

It has been a constant allusion that faster and bigger computers will provide the solution to many difficulties associated with the numerical integration of partial differential equations. Such larger and faster computers are needed but they do not provide the brutal force to resolve all the computational difficulties without conscientious efforts. Certain aspects of the problems must be understood as to their fundamentals before being satisfactorily dealt with, such as the questions of stability and accuracy. Moreover, the development of the computer hardware has reached the point through miniaturization that order of magnitude improvement in the speed of information processing cannot be expected as was in the past. The fourth generation computers promise to bring about large improvement in speed through "Parallelism" which is very much dependent on the sophistication of the software and on the nature of specific problems to be solved. They bring complicated problems to the users as well as to the manufacturer of the machines.

"Parallelism" is effected primarily in two different ways. Burrough Company's ILLIAC IV speeds up the arithematic process by using 64 arithematic units, receiving the same instruction from a common command module to process simultaneously 64 sets of raw data. Thus arithematic results can be "effectively" obtained 64 times faster. This is often referred to as a "single Instruction Multiple Processor" machine (SIMP). Control Data Corporation's STAR (the STring ARay processor) employs the assembly line or "pipe line" technique in which a string of data is "continuously" fed into the "pipe line" to be processed by a standing instruction. In this manner, the arithematic unit does not become idle when the instructions are being fetched, decoded, and installed in place to direct the

computation and when the newly computed data is being sent out of the arithematic unit or when the raw data is being brought into the arithematic unit. This is often referred to as the pipe-line machine. Both the ILLIAC IV and the STAR machines possess the virtual memory capacity, i.e., the machine will manage automatically the data stored in external memory units for extending the storage capacity of the machine. Texas Instrument Corporation's ASC machine (Advanced Science Computer) incorporates both the multi-processor and the pipe-line concept but possesses no virtual memory capability. All these machines are about to be (or already) delivered by the various manufacturers and are to become operational shortly.

ILLIAC IV is most efficient when the 64 arithematic processors can be fully utilized. Any vacant processors are simply idling, doing no useful work, when the operation is performed on less than 64 sets of data. Thus the demonstration of the speed of ILLIAC IV vs currently available computers is often in terms of the inversion of a 64 × 64 matrix. STAR is most efficient when a large number of raw data (the long string of data) is to be processed through the same operation so that the "filling time" of the pipe becomes negligible and the machine will provide a 64 time increase of the effective speed since each word in the STAR contains 64 bits of binary information. The ASC machine possesses intermediate behavior. Each manufacturer has developed powerful and intricate softwares to implement and enhance the advantages of the hardware. But all of them are subject to the inherent limitations of being a SIMP or a pipe-line machine.

For any one of these machines, a huge amount of data must be stored, arranged, and retrieved from storage facilities. They must be done efficiently, commensurate with the processing speed of the machine. Assume that such can be done for the data in core memory, directly accessible to the central processing unit (CPU), it cannot be done for the data stored in external memories. The speed of a search operation and of a data transmission through the interface to the CPU is orders of magnitude slower than the arithematic speed of the machine. If the CPU asks for data in the external storages too frequently, the CPU would be doing little useful computation but transmitting the data in and out of the external memory units under its virtual memory operation. If the user should prefer to deprive the machine of its virtual memory capability, then the user-programmer must assume the responsibility of managing the data across the interface. There is an alternative solution of this problem by expanding the core memory of the CPU of the computer to match its processing speed. This is unfortunately a very expensive proposition. There are also other problems of data management in the CPU, probably not so serious as the one just mentioned. They are more intimately related to the specific characteristics (hardware and software) of each computer. These are the problems which the user cannot help very much in its eventual solution. On the other hand, these machines present problems to the users, the solutions of which the manufacturer of the machines cannot help.

Currently available computers are serial machines that process and advance the data at one point after another. Simultaneous solution of unknowns at many points, as is required by implicit algorithms is handled through special procedures equivalent to matrix inversion. If a program designed for the serial machine should be run on the parallel computers,

no speed advantage will result. (Indeed there will be some loss.) The 64 parallel processors of ILLIAC IV will only have one processor doing useful work. The STring-ARray processor of STAR will operate in its scalar mode (versus the "vector mode" for string array processing).

There is not, and will not be, a software that will translate an existing serial program into a reasonably efficient "parallel program" for a specific parallel machine. Such a translation is not a matter of translating one language into another. It is a matter of changing the logic of solving a problem. It asks essentially for a new formulation for a specific problem to exploit the speed advantage offered by a specific machine. The user is asked to start anew, for each problem and for a specific computer and to pay considerable attention not only to the formulation of a problem for solution but also to the storage of the data in the external memory to match the demand of the data according to the formulation of the problem.

In writing such a program for use with a specific parallel computer, it is not a simple matter to take advantage of a successful serial program used with the current serial machines. It may indeed be doubtful, if there may be any advantage under special circumstances. Without further elaboration, it may be noted, even for simple problems, that:

- 1. An efficient serial algorithm need not lead to an efficient parallel algorithm while an inefficient serial algorithm may lead to an efficient parallel algorithm.
- 2. A serial algorithm that is apparently serial and was constructed for use with a serial computer may possess a great deal of hidden parallelism which may be exploited to suit the particular mode of operation of a specific parallel computer.

3. Parallel program may behave quite differently in the difference solution of a partial differential equation than the corresponding serial program. The behavior refers to the stability of the computation, the rate of convergence to the desired solution, and the accuracy of the solution.

The last one is particularly important. It asks the user to gain as much as possible the understanding of the various fundamental problems of difference methods such as stability and accuracy. With a better understanding, it may be hopeful that the years of todious and painful learning process through trial and error in developing the difference techniques of the serial machines may not be repeated or at least may be greatly reduced.

For many important practical problems the solution of the Navier-Stokes equations in three spatial dimensions will be required. Even for the steady state solution of such problems, the computation for a reasonably accurate solution will need the speed and storage capacity promised by these parallel computers. The complicated boundary conditions do not lend themselves to efficient parallel treatments and interfere with the efficient organization for the parallel computations of the fluid flow problems. This is in addition to the fundamental difficulties noted above. It is much desired that what has been learned from the serial machines may benefit the development of computational programs that will reap the promised speed advantage of the parallel computer. For this purpose, it is especially important to gain some fundamental understanding of such complicated computational difficulties special to fluid dynamics.

Such understanding cannot be expected from computer scientists who have their full share of difficulties associated with the operation of the parallel computers in general. Those wishing to solve the complicated flow problems with the Navier-Stokes equations must learn how to resolve such difficulties for themselves. The task shead is formidable. The potential reward is also immense.

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The mathematical foundation and the various practical aspects of the numerical solution of gas dynamic equations are critically reviewed with emphasis on obtaining quantitatively accurate solutions for application in various engineering and sciences Computational stability rate of convergence and accuracy (or error estimate) are discussed. The promises and problems of the 4th generation computers are outlined within this perspective.)

Computational stability should not be obtained at the sacrifice of the convergence rate to and the accuracy of the final solution. With accuracy in mind, the explicit algorithms are likely preferrable to the implicit ones. Strict conservation of the difference formulation is recommended and exemplified to avoid the accumulation of local truncation errors and to facilitate the estimate of the errors in a steady state solution. Illustrative examples are given including supersonic flows with shocks.

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